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TECHNICAL BACKGROUND DOCUMENT: INDUSTRIAL WASTE MANAGEMENT EVALUATION MODEL (IWEM), GROUND WATER MODEL TO SUPPORT THE GUIDE FOR INDUSTRIAL WASTE MANAGEMENT

DRAFT

April 13, 1999

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1.0 INTRODUCTION

EPA's Office of Solid Waste (OSW) is developing the ***Guide for Industrial Waste Management*** to facilitate evaluation of non-hazardous industrial waste (U.S. EPA, 1999). This document describes one aspect of the guidance, the technical basis for a ground-water model designed to determine if waste management unit (WMU) designs are protective of ground-water resources. The degree of ground-water protection provided by a particular design is determined by modeling the migration of waste constituents from the WMU through underlying soil to a monitoring point in an aquifer. The methodology and the assumptions used to perform the ground-water modeling and the application of the results of the modeling are described in this document.

This model incorporates two levels, or tiers, of analysis to provide facility managers, the public, and state regulators flexibility in assessing the protectiveness of particular WMU designs. The first level of analysis, Tier 1, is based on a conservative Monte Carlo probabilistic analysis that accounts for the nationwide variability of ground-water modeling parameters. Tier 1 requires minimal data about the facility and provides an analysis of the extent to which a WMU design or waste concentration for land application units protects ground water. The second level, Tier 2, allows users to change a subset of the facility-specific ground-water modeling parameters that may be known with greater certainty at a specific location. The Tier 2 analysis is based on a predictive neural network tool that incorporates the sophistication of a probabilistic ground-water modeling analysis yet requires a minimal amount of site data.

The unique aspect of the two-tiered approach developed by the Agency is that it provides two levels of analysis that require a minimum of data and provide instantaneous analysis and recommendations for the type of liner that should be used in a WMU and/or whether land application is appropriate. Both analyses are combined into a user-friendly Windows-based software tool, the Industrial Waste Evaluation Model (IWEM) that will operate on any standard, MS Windows™-based PC platform.

It should be noted here that the guidance also recommends detailed site-specific Tier 3 analysis in situations when a more thorough evaluation of site conditions is needed. This approach applies appropriate ground-water models and a full array of detailed site climatologic and hydrogeologic data. However, the Tier 3 analyses are beyond the scope of this background document and further information regarding their application to selecting appropriate liner designs for industrial solid waste management unit designs is described in the main ***Guidance*** (U.S. EPA, 1999).

The development of this two-tiered approach is described in detail in this document. The remainder of this section summarizes the objectives of the two-tiered approach and contains a list of the limitations, caveats, and disclaimers associated with the two-tiered approach used to evaluate Industrial WMU designs.

1.1 Objectives of this Document

The objectives of this document are to describe in detail the methodology and assumptions used to develop the two-tiered approach to evaluating WMU designs. Knowledge of the methodology and assumptions used to develop the two-tiered approach will allow the user, decision makers, and other stakeholders to determine if the approach is appropriate for the evaluation of specific WMU designs at specific sites.

This background document contains a summary of the overall modeling strategy used, a description of the models, the method used to calculate Tier 1 and Tier 2 leachate concentration threshold values (LCTVs), and a summary of how to apply the model results for Tier 1 and Tier 2 to the evaluation of WMU designs and waste concentrations for land application.

1.2 Relation to Other Documents

As stated above, this document describes the ground-water modeling methodology used to determine the protectiveness of a WMU design. Other aspects of the guidance, such as air emissions modeling and ground-water monitoring are described elsewhere in the main ***Guidance*** (U.S. EPA, 1999).

1.3 Limitations, Caveats and Disclaimers

The two-tiered approach developed to evaluate WMU designs uses the latest available peer-reviewed ground-water modeling methodology incorporating state-of-the-art probabilistic techniques to account for the uncertainty. However, given the complex nature of the evaluations, a number of limitations and caveats must be delineated. These are described in this section.

To perform the evaluations recommended by the ***Guide for Industrial Waste Management (Guidance)*** (U.S. EPA, 1999), mathematical models are used. These models are based on a number of simplifying assumptions to represent conditions that may potentially be encountered at waste management sites within the U.S. Efforts have been made to obtain representative nationwide data and account for the uncertainty in the data. However, as with all modeling evaluations, these simplifying assumptions potentially might not apply or may be inappropriate for evaluating a specific WMU design at a specific site with a unique combination of conditions that might not be accounted for with the available data. Therefore, where appropriate, EPA used conservative estimates of parameter values to ensure ground-water protection.

The two-tiered approach described in this document is designed to be used as guidance in the selection of an appropriate WMU design or land application of waste. Given the number of variables involved and the uncertainty of hydrogeologic characteristics of a specific site, the

application of this guidance is not intended to provide a guarantee that a specific design will be appropriate and protective. The fate and transport model upon which this analysis is based uses a national database. Evaluations using parameter values at the extremes of the distribution may have significant error associated with them.

The user, decision makers, and other stakeholders who are evaluating the results of a two-tiered analysis need to ensure that there is sufficiently documented and verifiable justification of site parameter values and any potential uncertainty or data gaps that may exist. This is especially true with respect to highly sensitive modeling parameters such as infiltration rate, WMU area, sorption and hydrolysis rates, and the distance to a ground-water monitoring well. Additional information about the uncertainty involved in the modeling and two-tiered approach is provided in Section 5.4 of this document.

The two-tiered approach presented in this document was developed by EPA in consultation with state regulatory agencies, representatives from industries, and environmental stakeholders. EPA has provided this guidance as a tool for states, industry, the public, and environmental groups, who may all have a role in making decisions regarding appropriateness of WMU designs.

2.0 OVERALL MODELING STRATEGY

This section describes the overall ground-water modeling strategy used to develop the two-tiered evaluations of WMU designs (Section 2.1). Section 2.2 presents a summary of the Monte Carlo analysis used in the ground-water modeling. Section 2.3 provides a summary of neural networks. The technical basis for the Tier 1 and Tier 2 approaches are described in sections 2.4 and 2.5.

2.1 Ground-Water Modeling Strategy

The development of a ground-water modeling strategy to evaluate WMU liner designs requires the development of a conceptual model to visualize what is being modeled. This conceptual model is used to select an appropriate ground-water fate-and-transport model and to outline underlying assumptions that will be used in the model. The following subsections describe the conceptual model and the three liner designs that will be considered in the two-tiered approach.

2.1.1 Conceptual Model

The approach used to evaluate the ground-water fate and transport component of contaminant releases from WMUs is illustrated by the conceptual model in Figure 2-1. Infiltration through the waste in the WMU depends on the climate characteristics (e.g., precipitation and evapotranspiration) and the WMU design (e.g., cover, liner, liquid or solid waste). Precipitation that percolates through the waste unit will generate leachate, which can infiltrate from the bottom of the WMU through the unsaturated zone and into the saturated zone and then downgradient to a ground-water receptor well that could be used to monitor unit performance or for drinking water. For purposes of the ***Guidance***, the well is considered a monitoring well. The fate and transport modeling computes the concentration of contaminants in this well, which is known as the ground-water or monitoring well.

The predicted contaminant concentration in the ground-water well is compared to a toxicity reference level; either maximum contaminant level (MCL) a health-based number (HBN). If the monitoring concentration of a contaminant is less than the toxicity reference level, a WMU design is considered to be protective of ground water.

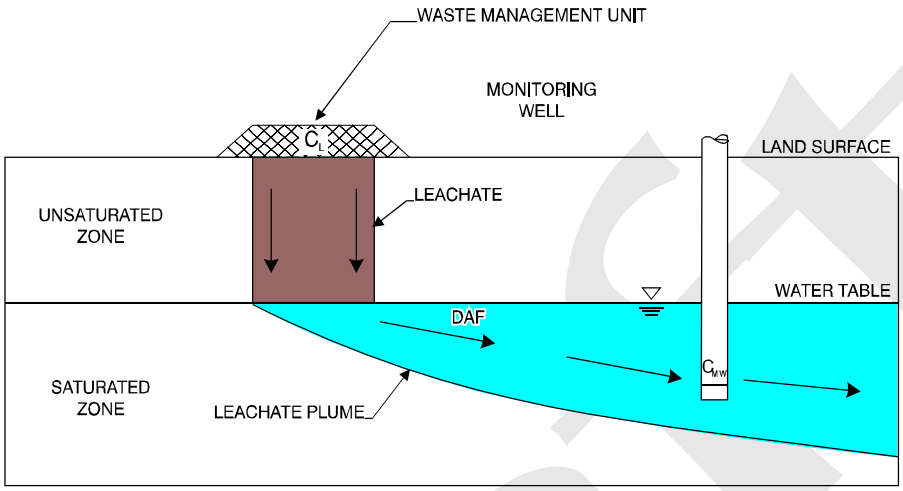

Figure 2-1 Schematic Diagram of Ground-Water Modeling Scenario

The objective of the ground-water modeling performed for this guidance is to compute the amount of dilution and attenuation a contaminant may undergo as it migrates from a WMU to a ground-water well. The amount of dilution and attenuation is expressed as a **dilution/attenuation factor (DAF)**, which represents the ratio of the **initial leachate concentration (C_L)** to the **ground-water monitoring well concentration (C_{MW})**:

$$DAF = \frac{C_L}{C_{MW}}$$

The DAF is assumed to be independent of the initial leachate concentration for most chemicals. For a given initial leachate concentration, there is a direct, one-to-one correspondence between DAF and monitoring well concentration. Therefore, computing a DAF for specific WMU scenarios allows for easy determination of the expected ground-water well concentration. The initial leachate concentration is divided by the DAF to determine the expected ground-water well concentration. Similarly, the toxicity reference level at the ground-water well represents an acceptable threshold value for the concentration of chemicals in ground water. Multiplying the toxicity reference level by the DAF produces an acceptable concentration level from a unit waste leachate. This acceptable leachate concentration is known as the **leachate concentration threshold value (LCTV)**.

The LCTV computed for a specific chemical for a given ground-water modeling scenario is compared to the leachate concentration of a waste of concern, as measured using the TCLP or other appropriate leaching test. If the leachate concentration is below the LCTV, the scenario modeled for the waste of concern will be protective of ground water.

LCTV = DAF * TRL

where:

LCTV = Leachate Concentration Threshold Value

DAF = Dilution/Attenuation Factor

TRL = Toxicity Reference Level *(e.g. MCL or HBN)*

The conceptual model described here is evaluated with a probabilistic ground-water model developed by the Agency, EPACMTP, EPA's Composite Model for Landfills with Transformation Products (U.S. EPA, 1996a). The probabilistic aspects of EPACMTP are summarized in Section 2.2. Additional details on specific EPACMTP modeling assumptions and parameter values and data sources are provided in Section 3.3.

2.1.2 Waste Management Unit liners

The primary method of controlling the release of waste constituents to the subsurface is to install a low permeability liner at the base of a WMU. A liner generally consists of a layer of clay or other material with a low hydraulic conductivity that is used to prevent or mitigate the flow of liquids from a WMU. However, the type of liner that is appropriate for a specific WMU is highly dependent upon a number of location-specific parameters, such as climate and hydrogeologic characteristics. In addition, the amount of infiltration of liquids from a WMU has been shown to be a highly sensitive parameter in predicting the release of contaminants to ground water. Therefore, one of the main objectives of the two-tiered modeling approach is to evaluate the appropriateness of a proposed liner design in the context of other location-specific parameters such as precipitation and evaporation and the characteristics of the subsurface beneath a facility.

EPA has chosen to evaluate three types of liner scenarios, the no-liner, single-liner, and composite-liner scenarios. The no-liner scenario (Figure 2a) represents a WMU that is relying upon location-specific conditions such as low permeability native soils beneath the unit or low annual precipitation rates to mitigate the release of contaminants to ground water. The single-liner scenario represents a 3 foot thick clay liner with a low hydraulic conductivity ($1x10^{-7}$ cm/sec) beneath a WMU (Figure 2b). The composite-liner scenario consists of a 3-foot-thick clay liner beneath a 40 mil thick high-density polyethyelene (HDPE) flexible membrane liner or FML (Figure 2c).

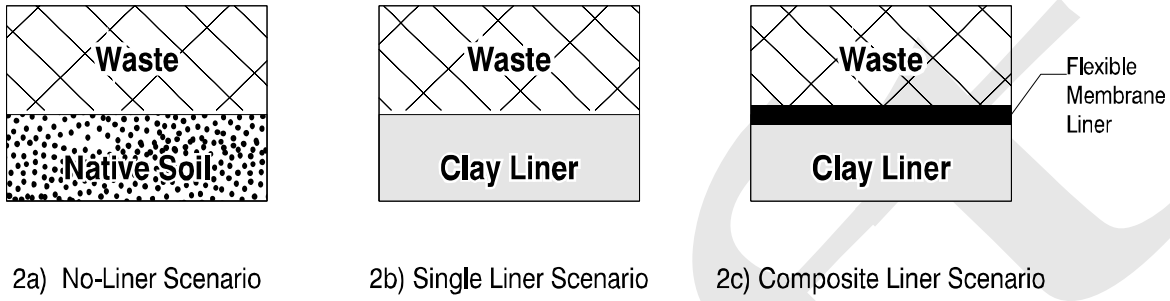

Figure 2-2 Three Liner Scenarios Considered in the Two-Tiered Modeling Approach for Nonhazardous Solid Waste Guidelines.

While other liner scenarios may be proposed by a facility or considered by the State authorities, such as double liners or liners with drainage layers and leachate collection systems, they are not addressed in the two-tiered approach described in this document. For further information on other liner scenarios, the reader is referred to the ***Guidance*** (U.S. EPA, 1999).

2.2 Monte Carlo Analysis

In its nationally applicable analyses of the fate and transport of waste constituents, the Agency for regulatory purposes, generally uses a Monte Carlo approach to compute probabilistic estimates of constituent concentrations in hypothetical downgradient ground-water wells. The Monte Carlo procedure randomly draws input parameter values from representative statistical distributions for each parameter (Figure 2-3). A set of input parameter values is developed and the model is run to compute the ground-water monitoring well concentration and the DAF. This process is repeated thousands of times until a distribution of thousands of output values (DAFs) is produced. The DAF values are ranked from high to low and for the purposes of the current ***Guidance***, the 90th percentile DAF is determined. The 90th percentile DAF represents the amount of dilution and attenuation that would occur in at least 90% of the cases modeled. Specifically, 90% of the DAF values would be greater than the 90th percentile DAF and 10% would be lower. In other words, the DAF is protective in at least 90% of the modeled cases. The use of the 90th percentile DAF therefore, provides a conservative measure of the amount of dilution and attenuation that would likely occur.

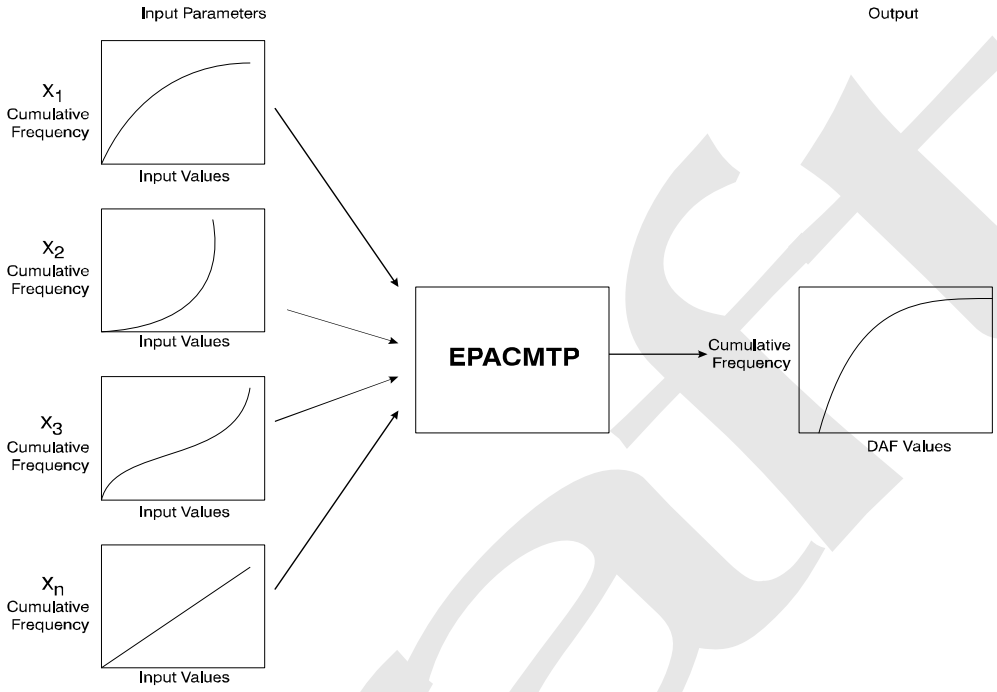

Figure 2-3 Schematic Diagram to Illustrate the Monte Carlo Modeling Approach

2.2.1 Basis for the Use of Monte Carlo Approach

Given the number of input parameters used in EPACMTP (52) and the application of EPACMTP to determine DAFs representative of waste management facilities nationwide, the output of the model, the DAF, may be subject to a high degree of variability and uncertainty. The Monte Carlo approach accounts for the variability (range of values) and uncertainty (level of confidence that the values are representative) in the input parameters by computing distributions of DAFs that are based on representative distributions of input parameters and reasonable and representative combinations of these input parameters.

The Monte Carlo approach used in EPACMTP has been applied in various EPA regulatory efforts, including the proposed Hazardous Waste Identification Rule (HWIR) of 1995 (U.S. EPA, 1995) and hazardous waste listing evaluations (for example, the Petroleum Refinery Waste Listing determination, U.S. EPA, 1997). As such, the Monte Carlo procedure and it's applicability to national analyses has been extensively reviewed within EPA and by the Science Advisory Board and has been subject to public review and comment.

2.2.2 Basis for Use of the 90th Percentile

The selection of a 90th percentile DAF (for DAFs ranked from highest to lowest) is based on the need to choose a level of protection that is conservative and consistent with other EPA analysis including the proposed 1995 HWIR and hazardous waste listing efforts mentioned above. Also, it is desirable to have a large degree of confidence that the results are adequately protective of human health and the environment given the degree of uncertainty inherent in the data and the analyses. Therefore EPA has selected the 90th percentile output of the ground-water fate and transport modeling for this guidance. The 90th percentile DAF implies that of the modeled scenarios (which are assumed to be representative of facilities nation wide) 90% result in DAFs that are higher than the 90th percentile DAF and thus are considered protective.

2.3 Development of Neural Networks to Emulate Ground-Water Models

To enable users to perform a ground-water modeling analysis to evaluate a WMU design, EPA developed a user-friendly method to obtain the results of other ground-water modeling analyses conducted by the Agency. The Agency generally uses EPA's EPACMTP ground-water fate and transport model analyses. However, because EPACMTP is a mechanistic model that runs in Monte Carlo mode, it requires up to several thousand iterations or realizations for each simulation to account for changes in parameter values. Each iteration uses one set of input parameter values that are randomly drawn from a representative statistical distribution. This process is repeated 2,000 times for each simulation to produce a statistical distribution of output values.

Therefore, even when EPACMTP is run on a current generation PC, such as a Pentium II, it requires up to several hours to complete a 2,000 iteration Monte Carlo simulation. In addition, EPACMTP is a complex model that requires ground-water modeling expertise and a large amount of facility and hydrogeologic data to be used effectively. Therefore, EPA developed a simplified easy-to-use version of EPACMTP for users with little or no ground-water modeling expertise and a minimum amount of key location-specific data. After exploring options, EPA chose to develop a neural network as a user friendly predictive tool that simulates EPACMTP and will compute a DAF based on user-defined values of 6 to 7 key EPACMTP input parameters.

A brief overview of what neural networks are and how they are used to evaluate Industrial WMU designs is provided in the following sections.

2.3.1 Brief Overview of Neural Networks

A neural network is a computational tool that can be used to predict outcomes based on the characteristics of multiple inputs to a function or a system. Neural networks generate a model to predict values of a variable (outputs) as a function of input data and can provide accurate predictions over wide ranges of input values for non-linear and non-Gaussian processes (SPSS, 1996). Many neural network models are similar or identical to popular statistical techniques such as generalized linear models, polynomial regressions, and nonparametric regressions (Sarle, 1994). Neural networks have been used in a number of real-world applications, including optimizing ground-water remediation strategies (Rogers, et al, 1995, Johnson and Rogers, 1995). Specifically, neural networks have been used in place of a mechanistic fate and transport model to determine the remediation success of various configurations of pumping wells to withdrawal and control of contaminant plumes (Rogers, et al, 1995). Neural networks also have been used to evaluate "what if" scenarios with Monte Carlo-style simulation experiments (Kalos and Whitlock, 1986). Other applications of neural networks to ground-water problems include prediction of aquifer parameters from geophysical curves (Aziz and Wong, 1992) and geospatial estimation of hydraulic conductivity (Rizzo and Daugherty, 1994).

Neural networks are developed with software that consists of a large number of simple computational or processing units (referred to as neurons) that are interconnected in a net-like structure. Software neural networks derive their terminology from their similarity to biological neural networks, such as the brain, in which the processing units are "neurons" that are interconnected. Both biological and software neurons receive input signals and send an output signal to other neurons in the network. The strengths of the connections between neurons, referred to as weights, can be changed in response to information provided to the neural network. As such, the network can learn and/or be "trained" to produce an output based on a set of inputs.

Neural networks are analogous to regression analysis, a statistical technique used to develop a best fit to observed data that can be used to predict an outcome based on a number of inputs. As stated above, each layer in a neural network consists of "nodes" (also known as neurons) and weights (Figure 2-4). The input nodes are the independent variables and the output nodes are the dependent variables. The hidden node values are analogous to regression equation terms and the weights are analogous to the coefficients in a regression equation. Neural networks are most often trained using least squares methods (Sarle, 1994), which involves minimizing the sums of squares of the error (similar to regression models) over all outputs.

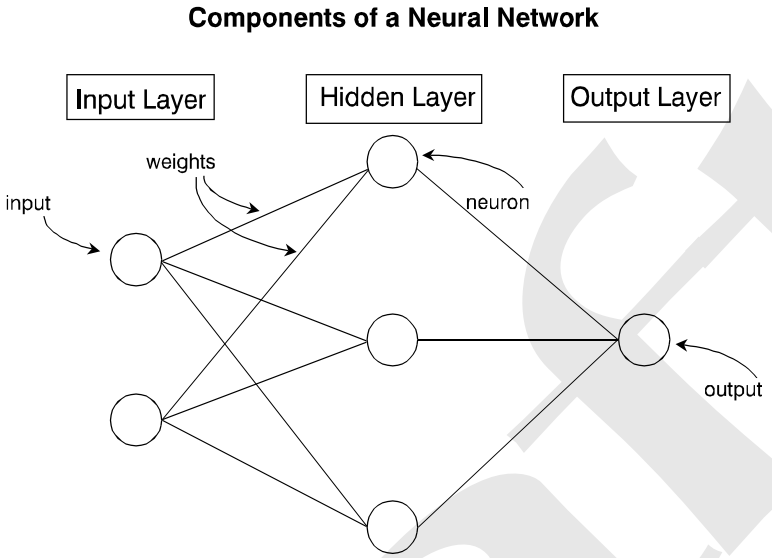

Figure 2-4 Schematic Diagram of a Neural Network

The neural network makes an initial prediction of what an outcome should be based on inputs it is given. It then computes the error, that is, the difference between the target (predicted) and actual (observed) values. Weights are then adjusted to reduce the errors and the neural network "backpropagates" to nodes within the network. Backpropagation involves working backward from the output node to adjust the weights accordingly, and reduce the average error across all nodes. This process is repeated until the weights reach their optimal values and the error in the output is minimized.

Components of Applying Neural Networks

The successful application of neural networks requires consideration of the following aspects, which are discussed below:

- Selecting an appropriate neural network architecture,
- Data pre-processing,
- Training,
- Performance evaluation

Many varieties of neural network architecture are available including multi-layer perceptrons (MLP), Radial Basis Functions (RBF), and Self Organizing Maps (Kohonnen networks) (SPSS, 1996). MLP networks are general-purpose, flexible, nonlinear models, based on the original models of neural computing (Sarle, 1994). MLPs (which are the architecture depicted in Figure 2-4) are suited to a wide range of applications, and currently are the most successful and widely used neural computing model (SPSS, 1996). For these reasons, EPA selected the MLP as the most appropriate architecture for developing neural networks for the ***Guidance***.

Pre-processing applies to any operations performed on the raw data to extract features relevant to a specific application, for example, natural log transformations and removal of outliers. For the Tier 2 neural network, log transformations were made of all input parameters and the output values (the DAF) to obtain values that were normally distributed.

The training or learning process consists of presenting the neural network with example data and then adjusting the network's internal weights until the desired response is obtained. The method used to adjust the weights is known as the training algorithm. Generally two types of training algorithms are used to develop neural networks: "supervised training" and "unsupervised training". In supervised training, the neural network learns to adjust its weights so that the outputs coincides with a particular target value. In unsupervised training, the neural network is not provided with a "target". Instead, it learns to recognize patterns inherent in the data. Given that the purpose of the neural networks was to predict a target DAF value, EPA used supervised training.

In general, increased numbers of training data sets and increased training iterations (the actual number of counts or times the weights are adjusted) will increase the predictive capability of a neural network. However, if a neural network is highly trained on data it has seen (training data sets), it might not be able to predict well using input data it has not been trained on. A key attribute of a trained neural network application is its ability to generalize (i.e., to give accurate answers on data that it did not "see" as part of the training process.) However, neural networks can become "over-fitted". An over-fitted neural network is one that produces excellent results with the training input data, but performs poorly when presented with data it has not seen before, even if it comes from the same source (i.e., the EPACMTP) as the training data. Such a neural network results in poor generalization. The achievement of good generalization is a key design aim, and it is achieved by careful choice of neural network size and the amount of training applied to the neural network.

Performance evaluation of neural networks consists of evaluating the ability of the trained network to predict an output based on inputs. A neural network's performance can be evaluated using standard R-squared statistics and plots of the actual outputs versus the neural network predicted outputs with 90% confidence intervals. Sensitivity analyses can be performed to determine the sensitivity of an output variable to changes made in input values. The results can be

ranked in order of decreasing sensitivity.

Selection of Appropriate Neural Network Training Software

Numerous neural network training software packages are available commercially and as shareware and freeware. For the purposes of the current ***Guidance***, a low-cost package called NNModel (Neural Fusion, Inc. 1998) was evaluated. NNModel was demonstrated to be an appropriate neural network modeling package for the purposes of developing the ***Guide for Industrial Waste Management*** based on it's ease of use, it's technical capabilities, low-cost, and ability to produce robust neural networks. Trial versions of the software are available on a shareware basis (http://www.neuralfusion.com/).

2.3.2 Development of a Neural Network to Emulate EPACMTP for Tier 2, Location-Adjusted Evaluations

To develop a neural network for the Tier 2 analysis for evaluations of Nonhazardous Solid Waste WMUs, the following steps were performed:

- EPACMTP was run to create training and test data sets;
- the EPACMTP output was imported to spreadsheets of modeling inputs and results;
- the spreadsheets were imported into NNModel and a data matrix was created;
- the data were examined with graphical visualization features of NNModel and appropriate transformations were performed to normalize the data;
- a neural network was created with the training and tested with test data sets; and
- the output for the neural network software is an exported neural network (ENN file), which is then linked to the windows-based graphical user interface.

For the Tier 2 analysis described in Section 2.6, a neural network was developed with the NNModel software and trained using sets of EPACMTP input and output parameter values. The trained network was used to predict the EPACMTP output value (the DAF) as a function of combinations of EPACMTP input values. The EPACMTP input parameters used to develop the trained neural networks are:

- area;
- infiltration;
- chemical hydrolysis rate;
- organic carbon partition coefficient;
- depth to water table;
- aquifer thickness; and
- distance to ground-water well.

Numerous combinations of various percentile values for each of these parameters were used to train the neural network (i.e., provide the neural network with the information necessary to predict the DAF based on changes in the values of these parameters). EPACMTP was run to develop a number of "training data sets" (sets of input and output parameter values) for combinations of these values, in which the DAF is the required output. Additional details of the neural networks developed for the Tier 2 analysis are provided in Section 5 and Appendix A.

2.4 Tier 1

For the Tier 1 National Evaluation modeling, the ground-water modeling scenario uses the conceptual model presented in Figure 2-1 (see section 3.3 for details of the assumptions used). The modeling assumptions used for three liner scenarios (shown in Figure 2-2) are the same for all chemicals considered, except for two chemical-specific parameters. The chemical-specific parameters, the organic carbon partition coefficient (K_{OC}) and the decay rate (λ), are used to determine the degree to which a chemical will sorb to subsurface soil particles and/or hydrolyze or otherwise breakdown into daughter chemical products, respectively. EPACMTP modeling was performed for the National Evaluation, and the results of this modeling are incorporated in tabular form in the IWEM software, providing Leachate Concentration Threshold Values (LCTVs) for all of the 190 Nonhazardous Solid Waste chemicals for liner scenarios for each type of WMU (with the exception that only the no-liner scenario is considered for land application units).

Given the large number of combinations of K_{OC} and λ for organic chemicals and the amount of time required to perform EPACMTP simulations for each of the organic constituents, EPA developed an interpolation procedure to reduce the amount of effort required to develop DAFs for organics. The process involved performing simulations for a range of representative combinations of K_{OC} and λ and interpolating between these values to obtain DAFs for the majority of the organic chemicals. This interpolation method and tests used to verify it are described in the EPACMTP Finite Source Methodology Background Document (U.S. EPA, 1996b).

The measure of how appropriate a liner design is for a particular WMU is determined by comparing the estimated waste constituent leachate concentration (as determined by the TCLP or other appropriate EPA test method) to the calculated LCTV in the appropriate Look-Up Table. This look-up function is performed automatically in the IWEM software. The result of this comparison determines the recommended liner system for the WMU or determines whether land application of this waste is appropriate and will not exceed the toxicity reference levels (i.e., health-based numbers or maximum contaminant levels) at a down gradient ground-water well.

For example, if the estimated leachate concentrations for all constituents are lower than the corresponding no-liner LCTVs, then the no-liner scenario is recommended as being sufficiently protective of ground water. If any leachate concentration is higher than the corresponding no-

liner LCTV, then a minimum of a single clay liner is recommended. If any leachate concentration is higher than the corresponding single-liner LCTV, then a minimum of a composite liner (an FML geomembrane overlain by a clay liner) is recommended. For waste streams with multiple constituents, the recommended liner design is based on the most protective liner required for any one constituent.

2.5 Tier 2

The Location-Adjusted Evaluation (Tier 2) is provided to assist the user in risk-based decision making regarding WMU liners or land application of waste. The Tier 2 Evaluation uses a set of four neural networks (one for each type of WMU) which enables the user to input certain location-specific data from a proposed or existing WMU. These location-specific data are then used to determine whether a liner is recommended as part of the WMU design for a given facility or to determine whether or not land application of a waste is protective of ground water.

Using a set of several thousand EPACMTP simulations, a neural network was trained for each type of WMU to estimate the DAFs that EPACMTP would have generated based on the values of the input parameters. The user can vary input parameter values within the range of values in EPACMTP's nationwide distributions, and the neural network then predicts the results that EPACMTP would have generated. Thus, the Location-Adjusted Evaluation allows the user to instantaneously evaluate a number of site-specific considerations without having to run EPACMTP or another ground-water fate and transport model. The Tier 2 neural networks mimic EPACMTP model results without requiring long simulation times. Additionally, the intuitive, windows-based user interface eliminates the need for the user to have training or extensive knowledge of neural networks, the EPACMTP model, or statistics. As is done in the National Evaluation, the expected waste leachate concentrations are compared to the Location-Adjusted LCTVs for the constituents of concern to determine the recommended liner type for the WMU or to determine whether land application of a waste is appropriate.

In developing and training the neural networks, problems were encountered when the extremes of the distributions were used as input to the training. Training of the neural networks was then limited to parameter values between the 10^{th} and 90^{th} percentile. The composite-liner infiltration rate assumed in Tier 1 (3×10^{-5} m/yr for landfills) was outside the 10^{th} to 90^{th} percentile range (0.024 to 0.45 m/yr for landfills), and thus the neural networks were not trained using this value. Because the use of infiltration rates outside the range over which the neural networks were trained will result in significant error, the Tier 2, Location-Adjusted Evaluation does not explicitly address the composite-liner scenario.

The proposed guidance still allows for assessment of the composite-liner scenario through the Tier 1 and Tier 3 evaluations. EPA is seeking comment on how to address inclusion of the composite-liner scenario in the Tier 2 Location-Adjusted Evaluation. One option currently under consideration is the development of multiple networks — one for low infiltration rates and one for high infiltration rates.

3.0 MODELS USED TO DEVELOP THE TWO-TIERED APPROACH

This section presents summary descriptions of the models used to develop the Tier 1 LCTVs and the Tier 2 neural networks. The following models were used:

- the HELP model for determining WMU infiltration rates;
- the MINTEQA2 model for determining metals sorption; and
- EPACMTP for determining dilution/attenuation factors (DAFs) of waste constituents in ground water.

Additional information can be found in the references cited in the description for each model. The software used to develop the neural networks for Tier 2 is discussed briefly in section 2.3.1 and additional detail on the development of neural networks is provided in Section 5.0.

3.1 HELP

The Hydrologic Evaluation for Landfill Performance (HELP) model is a quasi-two-dimensional hydrologic model used to compute water balance analyses of landfills, cover systems, and other solid waste management facilities (U.S. EPA, 1994). HELP uses weather, soil and design data and computes a water balance for landfill systems accounting for the effects of surface storage, snowmelt, runoff, infiltration, evapotranspiration, vegetative growth, soil moisture storage, lateral subsurface drainage, leachate recirculation, unsaturated vertical drainage, and leakage through soil, geomembrane or composite liners. HELP can model landfill systems consisting of various combinations of vegetation, cover soils, waste cells, lateral drain layers, low permeability barrier soils, and synthetic geomembrane liners. The model computes runoff, evapotranspiration, drainage, leachate collection and liner leakage that may be expected to result from the operation of a wide variety of landfill designs. The primary purpose of the model is to assist in the comparison of design alternatives.

3.1.1 Determining Infiltration from a Waste Management Unit

The HELP model requires that the user: input climatic data, using historical data provided for up to 101 cities in the U.S.; select the number of soil, waste and liner layers (e.g., liner, cover, waste layer, drainage layer) and the characteristics of each layer (thickness, hydraulic conductivity, etc.); and select surface characteristics (SCS Runoff Curve number, vegetative cover, and whether the layer is compacted). HELP uses these inputs to compute a water balance for the scenario selected by the user by computing the amount of precipitation that reaches the surface of the unit, minus the amount of runoff and evaporation. HELP then computes the amount of water that infiltrates through the surface layer (if applicable), into the waste layer, and through the bottom soil or liner, based on the initial moisture content and the hydraulic conductivity of each layer. The output

from the model is the amount of water that infiltrates through the bottom of the WMU. This value is then input to EPACMTP as the infiltration rate (in m/yr).

3.1.1.1 Determination of Surface Impoundment Infiltration Rate

The HELP model does not have the capability to estimate infiltration rates from surface impoundments. However, this capability is incorporated into EPACMTP. EPACMTP estimates the rate of infiltration through the base of the impoundment as a function of (1) the ponding depth of liquid in the waste unit, (2) the thickness of a low permeability sediment layer, or liner, at the base of the impoundment, and (3) the hydraulic conductivity of this impeding layer. Additional information regarding characterization and modeling of liquid wastes managed in surface impoundments is provided in the "EPACMTP Background Document and User's Guide" (U.S. EPA, 1996a).

3.1.2 Sensitivity of HELP Model to Input Parameter Values

As part of the evaluation of the applicability of the HELP model to the two-tiered approach, a sensitivity analysis was performed on the HELP model to determine the most sensitive, HELP input parameters (Allison Geoscience Consultants, Inc., 1997a). While the industrial waste guidance focuses its evaluation on the liner characteristics, this sensitivity analysis examined all HELP model input parameters to confirm the sensitivity of the liner characteristics. The sensitivity of the infiltration rate (computed with the HELP model) input to EPACMTP is discussed in Section 5.1

The sensitivity analysis quantitatively ranked HELP model input parameters based on their influence in determining the model's prediction of the infiltration rate of liquid from the bottom of a simulated landfill. The input parameters were restricted to a range of values expected in actual field designs and the analysis used a Monte Carlo shell program developed for EPA (Salhotra et al., 1988) linked with HELP. The Monte Carlo shell program linked to HELP enabled the specification of many of the HELP input parameters as probabilistic distributions rather than single, deterministic values. This allowed the parameter values to be random variables that take on new values each time the model is executed. The Monte Carlo shell supervises multiple executions of the HELP model, with each random variable assuming a new value for each execution. This can be likened to running the HELP model many times, with new values of the input parameters each time.

The probability distributions for each HELP input parameter limit the range of values the parameter can assume and even statistical properties that the set of generated parameter values should have, such as the mean and standard deviation. In this way, a large number of HELP simulations, each made with input parameters that have been randomly generated but constrained according to particular limits and statistical measures, are completed with a minimum of user

interaction. This large set of HELP simulations can be thought of as a set of deterministic model outcomes (or outcomes given some particular set of inputs). Each of the randomly generated model inputs was saved along with the model outcomes to determine which input parameters are most important in determining model outcome and the parameters were ranked according to their impact on the model output. This was accomplished by developing a correlation matrix that shows the statistical correlation between each model input parameter and the model outcome of interest.

The landfill scenario evaluated consisted of a closed landfill scenario with a cap consisting of a vegetative cover layer, a barrier layer, a waste layer, a lateral drainage layer with a leachate collection system, and a clay liner. Analyses were conducted for two representative sites, one in a humid region and one in an arid region of the U.S., based on climate data provided with the HELP model.

The sensitivity analysis indicated that the HELP model prediction of the average annual infiltration located in a relatively humid region (Atlanta, Georgia) is most sensitive to the following parameters:

1) the layer 1 (surface) soil textural and associated hydraulic properties,
2) the SCS runoff curve number,
3) the evaporative zone depth,
4) quality and quantity of vegetation maintained on the cover, and
5) the hydraulic properties of the cap barrier layer.

For the same design in an arid region (Las Vegas, Nevada) the model outcome is most sensitive to:

1) the evaporative zone depth,
2) the layer 1 soil textural and associated hydraulic properties, and
3) the quality and quantity of vegetation maintained on the surface.

The lack of rainfall in the model simulations for the arid case resulted in little or no moisture reaching the liner. This may have confounded the sensitivity analysis to the extent that the liner parameters for these scenarios have no impact on the results. This may suggest that in such dry regions the characteristics of the surface component of the landfill cap are very important in determining landfill performance.

Another conclusion of this sensitivity analysis applies not just to closed landfills, but to HELP's prediction of the performance of the bottom liner and leachate collection system. The percent of the infiltrate that passes through the cap of a landfill, or that migrates to the bottom liner in the case of an open landfill, and then percolates through the bottom liner, as predicted by HELP, is

determined by: 1) the hydraulic properties of the bottom liner and 2) the maximum drainage distance of the leachate collection system. Neither thickness of the liner or of the drainage layer, nor slope to the drains appears to be of much importance in HELP's estimate of this landfill performance measure. This conclusion is derived from analysis of the humid region results only, because of the lack of leachate that actually penetrated the cap barrier in the arid region case.

A related conclusion concerns the sensitivity of the model's prediction of the peak head on the bottom liner. That model outcome is most sensitive to: 1) the hydraulic properties of the bottom liner, 2) the maximum drainage distance of the leachate collection system, 3) the soil textural and hydraulic properties of the lateral drainage layer, and 4) the slope of the bottom layer in between the drains. This conclusion also is based only on the humid region modeling results, however, it would apply to the arid region scenario if a sufficient amount of liquid were to reach the bottom liner of the landfill.

The EPA acknowledges the importance of landfill design characteristics and the evaluation of drainage layers and leachate collection systems may most appropriately be considered in detailed Tier 3 analyses. However, the focus of the two-tiered approach is on the three liner scenarios described in Section 2.0. The HELP model sensitivity analysis confirms the primary importance of the hydrologic characteristics of the liners considered in Tier 1 and Tier 2.

3.2 MINTEQA2-derived and Empirical Isotherms

The process that most affects the transport of metals in the subsurface is sorption. The effect of sorption on metals transport is determined with sorption distribution coefficients. The sorption distribution coefficients (K_d) for metals used in the Tier 1 and Tier 2 scenarios are compatible with those used in other U.S. EPA regulatory efforts. The K_d values used in the modeling on which the Tier 1 approach is based are non-linear representations in which K_d is represented as a function of the total metal concentration and several important geochemical variables. The neural network used in the Tier 2 approach precluded the use of metal concentration-dependent K_d values. Therefore, empirical representations in which K_d is represented as a function of pH only were used. The methods use to model metals sorption are described in the following sections.

3.2.1 The K_d Values for Metals Used in Modeling Support for Tier 1

The K_d values for metals used in the modeling support for the Tier 1 approach were identical to those presented in U.S. EPA (1995). The K_d values were characterized in one of two ways, depending on the metal: 1) using empirical relationships that express K_d as a function of pH or 2) using the MINTEQA2 speciation model (Allison, et al, 1991).

Empirical relationships that express K_d as a function of pH were used (U.S. EPA, 1990) for the following metals:

- arsenic (As),
- antimony (Sb),
- chromium in the +6 oxidation state (Cr^{VI}),
- selenium (Se), and
- thallium (Tl).

The empirical pH-dependent relationships for these metals are shown in Table 3-1.

Table 3-1 Empirical pH-dependent K_d Relationships from U.S. EPA (1990).

Metal	K_d (liters kg^{-1})
As^{III}	$10^{(0.0322\ pH + 1.24)}$
Cr^{VI}	$10^{(-0.117\ pH + 2.07)}$
Sb^{V}	$10^{(-0.207\ pH + 2.996)}$
Se^{VI}	$10^{(-0.296\ pH + 2.71)}$
Tl	$10^{(0.110\ pH + 1.102)}$

For the following metals, the MINTEQA2 equilibrium speciation model was used to compute K_d as a function of metal concentration for specific settings of important system variables (pH, quantity of sorbent, etc.):

- barium (Ba),
- beryllium (Be),
- cadmium (Cd),
- chromium in the +3 oxidation state (Cr^{III}),
- copper (Cu),
- lead (Pb),
- mercury (Hg),
- nickel (Ni),
- silver (Ag),
- vanadium (V), and
- zinc (Zn).

The system-dependent, metal concentration-dependent K_d values computed with MINTEQA2 were then used in the unsaturated zone fate and transport modeling performed with EPACMTP.

The MINTEQA2 model and its use in determining the non-linear K_d relationships are described below.

Description of MINTEQA2

MINTEQA2 is an equilibrium speciation model developed and distributed by the U.S. EPA (Allison et al., 1991). For a particular metal, the model is used to calculate the equilibrium mass distribution among dissolved, sorbed, and precipitated phases. The input data for the model includes the pH, the major ion composition of the ground water, the expected concentration of dissolved and particulate organic carbon (DOC and POC), and an estimate of the concentration of binding sites associated with hydrous ferric oxide (HFO) of the solid aquifer matrix. The output from MINTEQA2 can be used to compute K_d. Specifically, for a particular metal, K_d is the ratio of total sorbed metal concentration to total dissolved metal concentration at equilibrium. A key assumption in using MINTEQA2 to compute K_d values for ground water is that the rate of chemical reactions, including sorption reactions, is fast relative to the ground-water flow velocity.

MINTEQA2

Input data:

- pH,
- the major ion composition of the ground water,
- the expected concentration of dissolved and particulate organic carbon (DOC and POC), and
- an estimate of the concentration of binding sites associated with hydrous ferric oxide (HFO) of the solid aquifer matrix.

Output:

- used to compute K_d, the ratio of total sorbed metal concentration to total dissolved metal concentration at equilibrium.

A typical K_d result computed by MINTEQA2 for Cd is shown in Figure 3-1. This result shows the variation in log K_d with the total cadmium concentration (log scale) for the case where pH is 6.8 and the concentrations of Cd binding sites associated with the DOC, POC, and HFO are all set to a mid-range value from a distribution of reasonable values. Details of the use of MINTEQA2 in computing K_d values used in Tier 1 modeling support are presented elsewhere (U.S. EPA, 1996c).

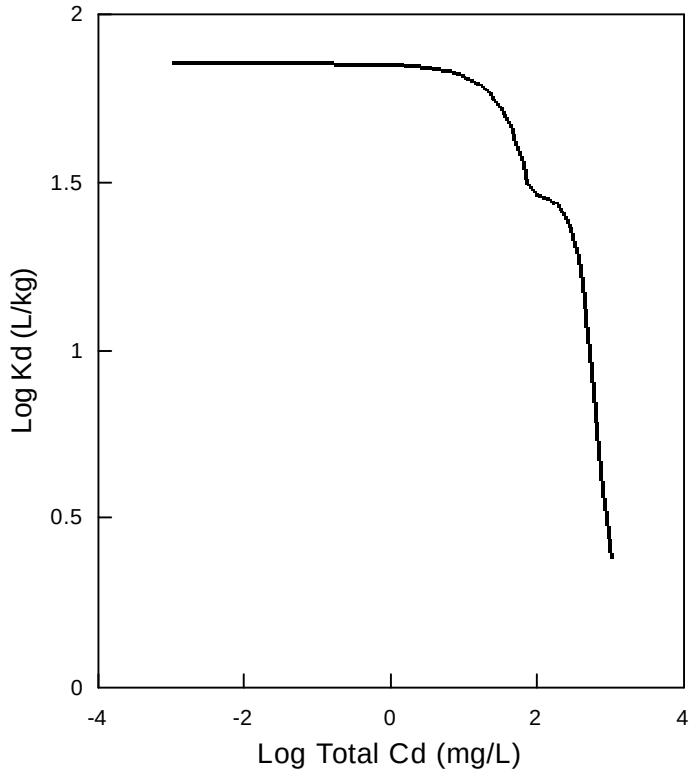

Figure 3-1 Variation in log K_d with log of Total Cd Concentration.

3.2.2 The K_d Values for Metals Used in the Neural Network for Tier 2

The K_d values for metals used in the neural network for Tier 2 are determined on the basis of pH. The pH-dependency for each metal is represented in the form of a regression equation of the form:

$$\log K_d = a(pH) + b \qquad \textbf{(2)}$$

as presented in U.S. EPA (1990). The empirically derived *a* and *b* parameters for this equation are shown in Table 3-2, as are representative values of K_d at pH 4.9, 6.8, and 8.0. The pH-dependent relationships whose parameters are shown in the table were determined from experimental analysis of aquifer material samples collected from across the U.S. The pH-dependent K_d relationships for As(III), Cr(VI), Sb(V), Se(IV), and Tl(I) have been used in other U.S. EPA regulatory efforts (e.g., U.S. EPA, 1995).

The metals Ag, Cr(III), and V were not included in the U.S. EPA (1990) study. For the tier 2 neural network, the pH-dependent relationship presented in Table 3-2 for Ni is also used for Ag, and the relationship for Cu is also used for Cr(III). Vanadium is assumed to be in the anionic form vanadate, which is modeled with the As(V) relationship from Table 3-2.

Development of the K_d values used in the Tier 2 Neural Network

The pH-dependent K_d relationships represented in Table 3-2 were determined from analyses of six aquifer material/ground-water samples. Aquifer material samples were added to ground-water samples to which metal had been added at concentrations ranging from 3 to 10 mg/L. After an equilibration period of 48 hours, the ground-water solution was extracted by centrifugation, and the metal concentrations remaining in solution were analyzed by inductively-coupled plasma spectrometry (ICP). In calculating K_d for a particular metal (M), the sorbed metal concentration (C_s) is equivalent to the difference between the total metal $[M]_{total}$ (after metal addition to the sample) and the metal remaining in the extracted supernatant solution $[M]_{solution}$ normalized by the concentration of solid aquifer material SC:

$$C_s = \frac{mg}{kg}\ \frac{[M]_{total}\ \frac{mg}{L} - [M]_{solution}\frac{mg}{L}}{SC\ \frac{kg}{L}} \qquad \textbf{(3)}$$

The equilibrium dissolved metal concentration (C_d) is equal to $[M]_{solution}$, so that K_d is determined with:

$$K_d \frac{L}{kg} = \frac{C_s}{C_d} \frac{mg/kg}{mg/L} = \frac{[M]_{total}\ mg/L - [M]_{solution} mg/L}{[M]_{solution}\ mg/l} \times \frac{1}{SC} \frac{1}{kg/L} \quad \textbf{(4)}$$

Experiments were conducted over a pH range of approximately 2 to 12. For each metal, the K_d values from Equation (3) were used in a linear regression analysis with pH as the independent variable. The parameters defining the resulting linear regression equations are those presented in Table 3-2.

Limitations of K_d Values Used in the Tier 2 Neural Network

The empirical pH-dependent K_d values of the U.S. EPA (1990) study are subject to uncertainty and to limitations and assumptions that arise from the experimental methods and the statistical analysis of the data. Most of the limitations result in increased likelihood of under-estimating sorption (and K_d) and increased uncertainty in the values. Certainly, the usual assumptions regarding equilibrium partitioning apply: the rate of partitioning of metal between the solution and solid phases was such that a close approach to equilibrium was achieved in the 48 hour equilibration period. If this was not the case, the K_d values may under-estimate actual partitioning. Also, the usual problems associated with filtering a sample to separate the solution and solid phases after equilibration contribute to uncertainty in the results. Other factors that should be taken into account when assessing these results include:

1. The $[M]_{solution}$ values used in Equation (3) did not always represent the actual concentration of metal remaining in solution. This is because of limitations of the ICP instrument used for this measurement. In cases where the concentration of metal remaining in solution was below the instrument detection limit, the value of $[M]_{solution}$ used in Equation (3) was set equal to the detection limit. This primarily impacted the value of the denominator in Equation (3). In cases where $[M]_{solution}$ was set to the detection limit, the resulting K_d was under-estimated. Different metals have different detection limits in this instrument, as detailed in U.S. EPA (1990).

Table 3-2 Regression Parameters of the pH-dependent K_d Relationships used in the Neural Network. (U.S. EPA, 1990).

Metal	*a*	*b*	K_d (L/kg)		
			pH 4.9	pH 6.8	pH 8.0
As(III)	0.0322	1.240±0.910	24.99	28.77	31.45
As(V)	-0.219	3.340±0.641	184.88	70.93	38.73
Ba	0.190	0.638±0.811	37.07	85.11	143.88
Be	0.378	-0.200±0.907	44.90	234.64	666.81
Cd	0.397	-0.943±0.820	10.05	57.10	171.00
Cr(VI)	-0.117	2.070±1.309	31.38	18.81	13.61
Cu	0.355	0.044±1.022	60.74	287.08	765.50
Hg	0.122	1.420±0.493	104.18	177.66	248.89
Ni	0.332	-0.471±0.797	14.32	61.18	153.11
Pb	0.0768	1.550±0.394	84.40	118.10	146.02
Sb(V)	-0.207	2.996±0.512	95.87	38.76	21.88
Se(IV)	-0.282	3.300±0.438	82.83	24.12	11.07
Se(VI)	-0.296	2.710±0.947	18.18	4.98	2.20
Tl(I)	0.110	1.102±0.542	43.75	70.79	95.94
Zn	0.378	-0.621±0.820	17.03	89.00	252.93

2. For a particular metal, the set of K_d values used in the statistical regression analysis included values that were calculated using $[M]_{solution}$ set to the detection limit. Thus, the resulting regression equations include the effects of under-estimates of K_d.

3. The ratio of solid aquifer material to solution was representative of a system with a low concentration of sorbing sites relative to the metal concentration. For a given metal concentration, such systems generally present a lower K_d than systems with a higher concentration of sorbing sites. The degree to which the resulting K_d values tend toward the conservative because of the ratio of sorbing sites to metal concentration is difficult to quantify.

4. For a particular metal, these K_d values were determined at one particular total metal concentration. Consequently, they do not represent the expected change in K_d with total metal concentration. These K_d values may be under-estimates in comparison with the actual K_d of the identical system with a lower total metal concentration. Conversely, they may be over-estimates of K_d in comparison with the actual K_d of the identical system with a higher total metal concentration.

3.2.3 Linear and Non-linear Sorption Isotherms

For a particular instance of transport modeling, the use of K_d values that vary with total metal concentration corresponds to the assumption of a non-linear metal sorption isotherm. The Tier 1 approach reflects the non-linear isotherm assumption. The use of a single K_d value (not dependent on metal concentration) in a particular instance of transport modeling, as is done in the neural network for Tier 2, corresponds to the assumption of a linear sorption isotherm. The assumption of a linear sorption isotherm is more realistic for metals that are not as strongly sorbed and for instances where the maximum total metal concentration is low.

Metals are adsorbed by soils and sediments at reactive sites on mineral and organic surfaces. A plot of sorbed metal concentration versus dissolved metal concentration at equilibrium is referred to as an isotherm, and the instantaneous slope of the isotherm plot is K_d. At low total metal concentration, the concentration of unreacted surface sites (i.e., those sites available to sorb metals) is much greater than the concentration of metal. If the total concentration of metal is increased, the system will respond by sorbing more metal. Moreover, the proportion of the added metal that is sorbed is essentially constant. Thus, K_d changes little so long as the concentration of unreacted sites is not significantly reduced. At higher metal concentrations, the concentration of unreacted sites begins to be depleted, and K_d for the system decreases more noticeably. For a particular metal at a particular total concentration of sorbing sites, the isotherm plot will show an almost linear trend (almost constant K_d) if only the low metal concentration portion of the curve is considered. The overall nature of the isotherm curve is non-linear, and this will be obvious if the portion extending to high metal concentration is considered. The instantaneous slope (K_d) can be

treated as approximately constant at low metal concentrations, but at higher metal concentrations, the slope changes considerably from the initial value.

The use of a single K_d corresponding to a linear isotherm has been favored in fate and transport modeling for metals because for most systems, too little data has been available to characterize the change in K_d with metal concentration, and because transport modeling is simplified by choosing a single value. The distinguishing feature of a non-linear isotherm is that it accounts for the depletion of available surface sites as successive pore volumes bring more metal into the system. This is important because, while the leachate concentration exiting a landfill or other source may not be very high, the total metal concentration in an equilibrating mass of aquifer in the subsurface will be equal to the leachate concentration only for the first pore volume. As adsorption occurs, successive pore volumes continue to bring in metal until the source is depleted. The total concentration of metal in the equilibrating mass of aquifer material will be the sum of the newly arriving leachate metal and the previously adsorbed metal from prior pore volumes. Depending on the initial K_d and the number of pore volumes of leachate that pass through, the total concentration of metal can become quite high, and the K_d may decrease due to depletion of unreacted sites.

Given the possible decrease in K_d in the subsurface with continued leaching, when it is necessary to use a single K_d for fate and transport modeling, a conservative value should be chosen. As can be seen from the foregoing discussion, the initial K_d of the pristine system is not a conservative value, rather, it is the maximum expected K_d. The single K_d values used in the Tier 2 approach represent values that have a conservative bias due to several factors (see discussion of limitations above). The ratio of solid sorbing sites to total metal concentration in the experiments from which these K_d values were determined contribute to the inherent conservatism of the values in a way that is difficult to assess.

3.3 EPACMTP

EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) is a fate and transport model used by EPA to establish regulatory levels for concentrations of chemicals in wastes managed in land disposal units (landfills, surface impoundments, waste piles, or land application units), for a number of EPA hazardous waste regulatory efforts. EPACMTP simulates one-dimensional, vertically downward flow and transport of contaminants in the unsaturated zone beneath a waste disposal unit as well as two-dimensional or three-dimensional ground-water flow and contaminant transport in the underlying saturated zone. The model accounts for the following processes affecting contaminant fate and transport: advection, hydrodynamic dispersion, linear or nonlinear equilibrium sorption, chained first-order decay reactions, and dilution from recharge in the saturated zone.

EPACMTP can be run in a probabilistic Monte Carlo mode (see Section 2.2) to randomly select parameter values from their respective statistical distributions. The Monte Carlo procedure allows assessment of the uncertainty associated with ground-water well concentrations that results from variations in the model input parameters.

The subsurface modeled by EPACMTP consists of a WMU, an unsaturated zone, and an underlying water table aquifer, and a ground-water well at a downgradient location in the aquifer (refer back to Figure 2-1). Contaminants move vertically downward from the base of the WMU through the unsaturated zone to the water table. EPACMTP allows simulation of flow and transport in the unsaturated zone and in the saturated zone, either separately or combined. For the two-tiered approach, the combined scenario was used.

EPACMTP consists of four major components:

- a module that performs one-dimensional analytical and numerical solutions for **water flow and contaminant transport in the unsaturated zone** beneath a WMU;
- a numerical module for **steady-state ground-water flow subject to recharge from the unsaturated zone**;
- a module of **analytical and numerical solutions for contaminant transport in the saturated zone;** and
- a **Monte Carlo module for randomly selecting input values** to account for the effect of variations in model parameters on predicted ground-water well concentrations

The model accounts for the following mechanisms affecting leachate constituent migration:

- leachate constituent transport by advection and dispersion,
- leachate constituent retardation resulting from reversible linear or nonlinear equilibrium adsorption onto the soil and aquifer solid phase, and
- chemical and biological degradation processes expressed as a first-order decay rate.

The latter may involve chain decay reactions if the contaminant or contaminants of concern form a decay chain. The assumptions and input parameters required to run EPACMTP for the majority of EPA ground-water evaluations are listed in Table 3-3. Modeling assumptions and input parameter values that are specific to computing infiltration rates for the ***Guidance*** are listed in Tables 4-1 through 4-3.

Table 3-3 EPACMTP Modeling Assumptions and Input Parameters

Overall Assumptions	
Modeling Element	Description or Value
Management Scenario	Landfill Surface impoundment Waste pile Land application unit
Modeling Scenario	Finite-source Monte Carlo; depleting source for organics, constant concentration pulse source for metals
Exposure Evaluation	Downgradient ground-water monitoring well; peak well concentration for noncarcinogens, maximum 30-year average well concentration for carcinogens; 10,000-year exposure time limit
Regulatory Protection Level	90 percent
Source Parameters	
Parameter	Description or Value
Waste Unit Area	Derived from Industrial D Waste Survey Data
Waste Unit Volume	User-specified
Infiltration Rate	
Landfill	Site-based, derived from water balance using HELP model
Surface Impoundment	Site-based, derived from impoundment depth using Darcy's law
Waste Pile	Site-based, derived from water balance using HELP model
Land Application Unit	Site-based, derived from water balance using HELP model
Leaching Duration	
Landfill	Derived from total mass of waste, continues until all constituents have leached out
Surface Impoundment	20 years (operational life of unit)
Waste Pile	20 years (operational life of unit)
Land Application Unit	40 years (operational life of unit)

Table 3-3 EPACMTP Modeling Assumptions and Input Parameters (cont'd)

Chemical-Specific Parameters:	
Parameter	Description
Decay Rate Organic Constituents Metals	 Hydrolysis constants compiled by U.S. EPA ORD No decay
Sorption Organic Constituents Metals	 K_{OC} constants compiled by U.S. EPA ORD MINTEQA2 sorption isotherm coefficients for [Pb, Hg (II), Ni, Cr (III), Ba, Cd, Ag, Zn, Cu (II), Be]; pH-dependent isotherm coefficients for [As (III), Cr (VI), Se (VI), Th]
Unsaturated Zone Parameters	
Parameter	Description
Depth to Ground water Soil Hydraulic Parameters Fraction Organic Carbon Bulk Density	Site-based, from API/USGS hydrogeologic database ORD data based on national distribution of three soil types (sandy loam, silt loam, silty clay loam) ORD data based on national distribution of three soil types (sandy loam, silt loam, silty clay loam) ORD data based on national distribution of three soil types (sandy loam, silt loam, silty clay loam)
Saturated Zone Parameters	
Parameter	Description
Recharge Rate Saturated Thickness (depth to water table) Hydraulic Conductivity Hydraulic Gradient Porosity Bulk Density Dispersivity Ground-water Temperature Fraction Organic Carbon pH	Site-based, derived from regional precipitation and evaporation: and soil type Site-based, from API and USGS hydrogeologic database Site-based, from API and USGS hydrogeologic database Site-based, from API and USGS hydrogeologic database Effective porosity derived from national distribution of aquifer particle diameter Derived from porosity Derived from distance to ground-water well Site-based, from USGS regional temperature map National distribution, from U.S. EPA STORET database National distribution, from U.S. EPA STORET database

Table 3-3 EPACMTP Modeling Assumptions and Input Parameters (cont'd)

Ground-Water Well Parameters	
Well Element	Description
Radial Distance From WMU	Nationwide distribution, from U.S. EPA screening survey (U.S. EPA, 1987)
Angle Off-Center	Uniform within ± 90E from plume center line (no restriction within plume)
Depth of Intake Point	Uniform throughout saturated thickness of aquifer

Notes:
API = American Petroleum Institute
HELP = Hydrologic Evaluation Landfill Performance
ORD = Office of Research and Development
USGS = United States Geological Survey
STORET = Data Base Utility for the Storage and Retrieval of Chemical, Physical, and Biological Data for Water Quality.
For Additional information on EPACMTP data sources, see U.S. EPA (1996a, 1996b, and 1996c).

3.3.1 Analysis of Unsaturated Zone and Saturated Zone Flow and Transport

The method used in EPACMTP to analyze flow and transport in the unsaturated and saturated zones is described as follows:

Flow in the Unsaturated Zone. Flow in the unsaturated zone is assumed to be steady-state, one-dimensional vertical flow from beneath the source toward the water table. The lower boundary of the unsaturated zone is assumed to be the water table. The flow in the unsaturated zone is predominant gravity-driven, and therefore the vertical flow component accounts for most of the fluid flux between the source and the water table. The flow rate is assumed to be determined by the long-term average infiltration rate through the WMU. In surface impoundments, the flow rate is assumed to be determined by the average depth of ponding.

Transport in the Unsaturated Zone. Contaminant transport in the unsaturated zone is assumed to occur by advection and dispersion. The unsaturated zone is assumed to be initially contaminant-free, and contaminants are assumed to migrate vertically downward from the disposal facility. EPACMTP can simulate both steady-state and transient transport in the unsaturated zone with single-species or multiple-species chain decay reaction, and with linear or nonlinear sorption.

Flow in the Saturated Zone. The saturated zone module of EPACMTP is designed to simulate flow in an unconfined aquifer with constant saturated thickness. The model assumes regional flow in a horizontal direction with vertical disturbance resulting from recharge and infiltration from the overlying unsaturated zone and waste disposal facility. The lower boundary of the aquifer is assumed to be impermeable. Flow in the saturated zone is assumed to be steady-state.

EPACMTP accounts for different recharge rates beneath and outside the source area. Ground water mounding beneath the source is represented in the flow system by increased head values at the top of the aquifer. This approach is reasonable as long as the height of the mound is small relative to the thickness of the saturated zone.

Transport in the Saturated Zone. Contaminant transport in the saturated zone is assumed to be a result of advection and dispersion. The aquifer is assumed to be initially contaminant-free, and contaminants are assumed to enter the aquifer only from the unsaturated zone immediately underneath the waste disposal facility, which is modeled as a rectangular, horizontal plane source. EPACMTP can simulate both steady-state and transient three-dimensional transport in the aquifer. For steady-state transport, the contaminant mass flux entering at the water table must be constant with time; for the transient case, the flux at the water table may be constant or may vary as a function of time. EPACMTP can simulate the transport of a single-species or multiple-species subject to chain decay reactions, and linear or non-linear sorption.

EPACMTP also accounts for chemical and biological transformation processes. All transformation reactions are represented by first-order decay processes. An overall decay rate is specified for the model; the model cannot explicitly consider the separate effects of multiple degradation processes such as oxidation, hydrolysis, and biodegradation. The user must determine the overall, effective decay rate when multiple decay processes are to be represented. EPACMTP also has the capability of determining the overall decay rate from chemical-specific hydrolysis constants using soil and aquifer temperature and pH values. EPACMTP assumes that reaction stoichiometry is prescribed for scenarios involving chain decay reactions. The speciation factors are specified as constants by the user (see the "EPACMTP Background Document and User's Guide", U.S. EPA, 1996a). In reality, these coefficients may change as functions of aquifer conditions (for example, temperature and pH), concentration levels of other chemical components, or both.

3.3.2 Data Sources

Data were obtained from a nationwide survey of industrial non-hazardous WMU's (landfills, surface impoundments, waste piles, and land application units) (Westat, 1987) to characterize WMUs and hydrogeologic characteristics at facilities nationwide. Parameters and assumptions used to estimate infiltration of leachate from each type of WMU are provided in the "EPACMTP Background Document and User's Guide" (U.S. EPA, 1996a).

3.3.3 Model Sensitivities to Input Parameters

Given the large number of EPACMTP input parameters (52) and the variability and wide ranges of values for some input parameters, EPA's objective in developing the two-tiered approach was to focus on the most important or most sensitive input parameters (i.e., those parameters whose

values would have the greatest impact on the output of EPACMTP). Focusing on the most sensitive parameters minimizes the amount of data required to perform an analysis while maintaining the robustness of the analysis.

The most sensitive input parameters were identified by performing sensitivity analyses which consisted of running EPACMTP with high and low values of each input parameters and looking at the resultant difference in the output (the DAF). Three separate sensitivity analyses were conducted:

1) a deterministic analysis of high and low values of input parameters;
2) a probabilistic analysis of high and low values of input parameters; and
3) a probabilistic analysis of the linear and rank order correlation coefficients to determine sensitivities of input parameters (Allison Geoscience Consultants, Inc., 1997b).

These three types of sensitivity analysis were performed and the combined results used to best determine the list of most sensitive parameters. As is described in the summary of each analysis, subtleties in the model sensitivity for probabilistic runs might only become apparent in a deterministic sensitivity analysis. However, probabilistic sensitivity analysis were needed because the modeling for Tier 1 and Tier 2 is probabilistic. The two different probabilistic sensitivity analyses were performed to provide independent confirmation of the sensitivity of input parameters for probabilistic modeling analyses.

The list of 52 EPACMTP input parameters to evaluate in the sensitivity analyses was reduced to 28 by identifying the independent variables that directly affect the EPACMTP output (well concentration). The 24 parameters not evaluated are either parameters included in the model to consider additional fate and transport phenomenon, but not used for the scenarios of interest to this analysis, dependent variables, or fixed (constant) values. Each of these parameters was not evaluated because they are not used for this analysis or are held constant and therefore have no impact on the model output.

A deterministic sensitivity analysis described in the following section was performed to determine the ranked sensitivity of each of these 28 parameters (Table 3-4).

Table 3-4 List of 28 EPACMTP Input Parameters Used in the Deterministic Sensitivity Analysis.

Variable	Code Name	Median Value	Units
Infiltration	SINFIL	0.18	m/yr
Recharge	RECH	0.168	m/yr
WMU area	AREA	4.21	m^2
Depth of landfill	DEPTH	2.6	m
Fraction of industrial waste in landfill	FRAC	0.5	unitless
Density of industrial waste	CTDENS	0.9	g/cm^3
pH of ground water	PH	6.8	unitless
Temperature of ground water	TEMP	14.4	^oC
Dissolved phase hydrolysis decay rate	RLAM1	0.06	1/yr
Sorbed phase hydrolysis decay rate.	RLAM2	0.06	1/yr
Average particle diameter of aquifer material	DIAM	0.025	cm
Unsaturated zone thickness (depth to water table)	DSOIL	1.17	m
Residual water content of unsaturated zone	WCR	0.07	unitless
Soil bulk density	RHOB	1.65	g/cm^3
Soil moisture parameter	ALPH	0.0153	1/cm
Soil moisture parameter	BETA	1.37	unitless
Unsaturated zone hydraulic conductivity	SATK	0.091	cm/hr
Aquifer Thickness	ZB	1.182	m
Hydraulic conductivity of aquifer	XKX	3.2	m/yr
Ground-water hydraulic gradient	GRAD	0.0057	m/m
Porosity	POR	0.236	unitless
Longitudinal dispersivity of aquifer	AL	7	m
Organic Carbon Partition Coefficient	KOC	0.8	ml/g
Percent organic matter	POM	0.8	ml/g
Fraction Organic Carbon	FOC	0.00043	ml/g
Angle of well off plume centerline	ANGL	45	degrees
Radial distance to downgradient well	RADIS	427	m
Depth of well intake point (fraction of aquifer	ZWELL	0.5	unitless

Deterministic Sensitivity Analysis

Deterministic sensitivity analyses of the EPACMTP evaluated the effects of changes in single values of input parameters on a single output value. The deterministic sensitivity analysis evaluated the impact on predicted ground-water well concentration as a function of changing each parameter from it's 10^{th} to 90^{th} percentile value while holding other parameters at their 50^{th} percentile values.

The advantage of the deterministic sensitivity analysis is that it allowed the isolation of sensitive parameters that might be masked in Monte Carlo runs and might not reveal how sensitivities are dependent upon values of other parameters (e.g., whether or not contaminant degradation is considered, as described above). The disadvantage of the deterministic sensitivity analysis is that it might not reveal sensitivities or interdependencies that are representative of the probabilistic modeling required to evaluate industrial waste management scenarios.

For example, the deterministic analysis of longitudinal hydraulic conductivity of the saturated zone (XKX) indicated that it was not a sensitive parameter. However, closer examination reveals that at low values of XKX, the contaminant travels so slow that it does not reach the ground-water well, resulting in a low C_{MW}. At high values of XKX, the contaminant is transported rapidly but is highly diluted, also resulting in a low concentration C_{MW}. The highest C_{MW} values are actually reached at median values of XKX. Therefore, due to the design of the deterministic sensitivity analysis, XKX was not determined to be a sensitive parameter (i.e., there was an insignificant difference in the output for high and low values of XKX). However, based on other modeling analyses and knowledge of the importance of advection in groundwater flow and transport, hydraulic conductivity is generally recognized as a sensitive parameter.

The results of the deterministic sensitivity analysis identified a ranking of parameters in terms of model sensitivity. Those parameters that ranked on the bottom list were evaluated and determined to be parameters that generally are not sensitive for the modeling scenarios considered for the two-tiered analysis. Those parameters that are not sensitive for the scenarios of interest to the two-tiered approach are:

- FRAC - the fraction of the waste of concern in the landfill;
- DEPTH - the depth of the landfill;
- CTDENS - the density of the waste of concern in the landfill;
- pH - pH of the ground water;
- TEMP - ground-water temperature;
- RECH - aquifer recharge rate; and
- RLAM2 - a secondary parameter used to express first-order decay.

Probabilistic Sensitivity Analyses

The intent of the ***Guidance*** is to incorporate the probabilistic aspect of EPACMTP while focusing on those parameters that have the greatest impact on the model results. Therefore, probabilistic sensitivity analyses also were performed to identify sensitive parameters when EPACMTP is run in Monte Carlo mode. The probabilistic sensitivity analysis evaluated the effects of changes in one input parameter and holding that parameter at one value while using Monte Carlo values for the remaining parameters for thousands of iterations per simulation. The probabilistic sensitivity analysis determined the effect of changes in a single input parameter value on the statistical distribution of output ground-water well concentrations. For the purposes of the ***Guide for Industrial Waste Management***, which evaluates the 90th percentile output of EPACMTP, the probabilistic sensitivity analyses evaluated the effects of changes in one parameter on the 90th percentile ground-water well concentrations.

The sensitivity of EPACMTP to key input parameters for probabilistic simulations was evaluated to identify sensitive parameters with which to develop a neural network. Monte Carlo simulations were performed for the four types of WMUs: landfills, surface impoundments, waste piles, and land application units. As a result of the large amount of time required to perform a probabilistic sensitivity analysis on each of the 28 parameters for each of the four WMUs, the analysis focused on a subset of the parameters identified as the most sensitive in the deterministic sensitivity analysis:

- Source Specific parameters
  - area of disposal unit (AREA);
  - infiltration rate from disposal unit (SINFIL);
- Chemical-specific properties
  - hydrolysis rate (RLAM1);
- Unsaturated zone properties
  - thickness of unsaturated zone (DSOIL);
- Aquifer properties
  - longitudinal hydraulic conductivity (XKX);
  - hydraulic gradient (GRAD);
  - aquifer thickness (ZB);
- Ground-water well location
  - radial distance of the observation well from center of downstream edge of waste disposal unit (RADIUS); and

- **S** angle off-center of observation well measured counterclockwise (ANGLE).

The method used to perform probabilistic sensitivity analyses involved performing Monte Carlo (probabilistic) simulations to compute the "relative difference" between the output for a low input parameter value and the output for a high input parameter value. To examine the sensitivity of one parameter, one series of probabilistic simulations was performed to determine the "base case" (all input parameter values selected via Monte Carlo procedure) EPACMTP output value. Another series of probabilistic simulations was performed to determine the output value for a "low" (10^{th} percentile) input value of each parameter. A third series of probabilistic simulations was performed to determine the output value for a "high" (90^{th} percentile) input value of each parameter.

The sensitivity of some of the EPACMTP input parameters is dependent upon the values of other parameters. For example, if the angle of the ground-water well off the plume centerline is held at a high value (e.g., 90^{o}), the ground-water well will more likely be located outside of the contaminant plume. Therefore, the concentration in the ground water will likely be zero regardless of changes in values of any other parameters. The sensitivity of parameters also is dependent on whether or not contaminant degradation (sorption/hydrolysis) is considered. For example, if adsorption and hydrolysis are not considered, changes in the depth of the unsaturated zone (and other contaminant degradation-related parameters) will have no effect on the ground-water well concentrations.

The results of the ranked probabilistic sensitivity analysis are shown in Tables 3-5 and 3-6. The ranked order of the most sensitive parameters reflect both the spread in the input distribution of each parameter and the intrinsic sensitivity of that parameter. In other words, input parameters with a high degree of variation between their low and high values will tend to show a higher sensitivity than parameters with a low degree of variation. WMU area consistently shows a high ranking, because it has a wide frequency distribution and because changes in the source area will directly affect the predicted ground-water well concentration.

Additional observations from the sensitivity analysis are summarized as follows.

- As a general trend for the four types of management units, **the ground-water well location (ANGLE and RADIS) and the source area (AREA) most strongly influence the results**. The rate of **water infiltration through the source (SINFIL) is among the most sensitive parameters for landfills and land application units**, while it is less so for surface impoundments and waste piles. For surface impoundments, the rate of leakage from the waste unit is controlled primarily by the operating depth of the impoundment (HZERO) and the permeability and thickness of an impending layer at the base of the impoundment, but natural precipitation has little impact.

Table 3-5 Ranked Sensitivity of Parameters Evaluated in Probabilistic Sensitivity Analysis for (a) Landfills, (b) Surface Impoundments.

(a) Landfills

Decay Rate (l) = 0 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.01 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.1 yr^{-1}	Sensitivity Rank
Area	6.85	Area	8.07	Area	22.80
Infiltration	3.62	Infiltration	4.02	Infiltration	8.79
Radial Distance to Well	3.20	Angle of Well off of Plume Centerline	3.59	Angle of Well off of Plume Centerline	7.43
Angle of Well off of Plume Centerline	3.19	Radial Distance to Well	3.54	Radial Distance to Well	7.07
Hydraulic Conductivity	1.69	Aquifer Thickness	1.47	Aquifer Thickness	2.78
Hydraulic Gradient	1.22	Hydraulic Conductivity	1.39	Depth of Unsaturated Zone	2.67
Aquifer Thickness	1.17	Hydraulic Gradient	1.05	Hydraulic Conductivity	0.94
Depth of Unsaturated Zone	0.01	Depth of Unsaturated Zone	0.61	Hydraulic Gradient	0.24
Depth of Landfill	0.01	Depth of Landfill	0.61	Depth of Landfill	0.00

(b) Surface Impoundments

Decay Rate (l) = 0 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.01 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.1 yr^{-1}	Sensitivity Rank
Angle of Well off of Plume Centerline	6.61	Angle of Well off of Plume Centerline	7.84	Radial Distance to Well	20.19
Radial Distance to Well	6.30	Radial Distance to Well	7.75	Angle of Well off of Plume Centerline	15.94
Area	5.89	Area	7.17	Area	12.64
Hydraulic Conductivity	2.48	Aquifer Thickness	2.84	Ponding Depth	5.93
Aquifer Thickness	2.47	Ponding Depth	2.79	Aquifer Thickness	5.37
Ponding Depth	2.34	Hydraulic Conductivity	2.20	Depth of Unsaturated Zone	4.09
Hydraulic Gradient	2.01	Infiltration	2.14	Infiltration	4.05
Infiltration	1.93	Hydraulic Gradient	1.32	Hydraulic Conductivity	1.30
Depth of unsaturated zone	0.47	Depth of unsaturated zone	0.88	Hydraulic Gradient	0.24

Table 3-6 Ranked Sensitivity of Parameters Evaluated in Probabilistic Sensitivity Analysis for (a) Waste Piles, and (b) Land Application Units.

(a) Waste Piles

Decay Rate (l) = 0 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.01 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.1 yr^{-1}	Sensitivity Rank
Angle of Well off of Plume Centerline	34.2	Angle of Well off of Plume Centerline	32.7	Angle of Well off of Plume Centerline	5.46
Area	27.3	Area	25.5	Radial Distance to Well	5.27
Radial Distance to Well	23.0	Radial Distance to Well	24.0	Area	4.17
Hydraulic Conductivity	6.09	Aquifer Thickness	4.89	Aquifer Thickness	1.34
Aquifer Thickness	4.85	Hydraulic Conductivity	4.79	Infiltration	0.42
Hydraulic Gradient	2.82	Infiltration	1.88	Depth of unsaturated zone	0.30
Infiltration	1.86	Hydraulic Gradient	1.87	Hydraulic Conductivity	0.30
Depth of unsaturated zone	0.40	Depth of unsaturated zone	0.8	Hydraulic Gradient	0.12

(b) Land Application Units

Decay Rate (l) = 0 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.01 yr^{-1}	Sensitivity Rank	Decay Rate (l) = 0.1 yr^{-1}	Sensitivity Rank
Area	2.55	Area	3.38	Infiltration	11.6
Radial Distance to Well	2.37	Radial Distance to Well	2.92	Area	8.39
Infiltration	1.78	Infiltration	2.75	Radial Distance to Well	7.82
Aquifer Thickness	1.49	Aquifer Thickness	1.88	Angle of well off of plume centerline	6.00
Hydraulic Conductivity	1.18	Depth of unsaturated zone	1.21	Depth of unsaturated zone	5.26
Hydraulic Gradient	0.68	Hydraulic Conductivity	1.05	Aquifer Thickness	2.54
Angle of well off of plume centerline	0.58	Angle of well off of plume centerline	0.97	Hydraulic Conductivity	1.38
Depth of unsaturated zone	0.42	Hydraulic Gradient	0.40	Hydraulic Gradient	0.03

C The relative ranking of the four most sensitive parameters (ANGLE, RADIUS, AREA, AND SINFIL) is not the same for all four types of WMUs because the source specific parameters (AREA and SINFIL) have different ranges of values for each of the different WMUs. For example, 50th percentile values of area for the four WMUs are:

landfills	18,500 m^2
surface impoundments	2,685 m^2
waste piles	405 m^2
land application units	80,900 m^2

- Model results are highly sensitive to the location of the ground-water well, because the choice of the well location affects the concentration that will be measured at that location. Additionally, the ground-water well location increases in importance as the contaminant degradation (i.e., sorption and/or hydrolysis) rate increases. For example, as the hydrolysis rate increases, well location becomes even more critical because the contaminant will hydrolyze and will not travel as far as a conservative (non-hydrolyzing) contaminant.

- As the hydrolysis rate increases, the thickness of the unsaturated zone (DSOIL) and aquifer thickness (ZB) increase in importance, and the hydraulic conductivity (XKX) and gradient (GRAD) decrease in importance.

- For hydrolyzing constituents, the contaminant concentration reaching the ground-water well is highly dependent on the travel time (in both the unsaturated zone and the aquifer). The travel time, in turn, is controlled by the total travel distance (through the unsaturated and saturated zones) and the travel velocity. Thus the unsaturated zone thickness (DSOIL) and aquifer thickness (ZB) increase in relative importance to other parameters as hydrolysis rate increases.

- The travel velocity in the saturated zone is a function of the aquifer hydraulic conductivity (XKX) and hydraulic gradient (GRAD). It may, therefore, seem inconsistent that the sensitivity of these two parameters would decrease at higher hydrolysis rates. This apparent inconsistency highlights the fact that very complex interactions in the subsurface environment control the ground-water well concentration.

- The effect of increasing ground-water flow rate (by increasing either the hydraulic conductivity or the hydraulic gradient) results in a shorter travel time, and in the case of degraders, higher ground-water well concentrations. On the other hand, an increased ground-water flow rate also will cause a greater degree of dilution and dispersion of the contaminant, which will tend to lower the ground-water well concentration. The effects

of dilution will be more important for non-degrading constituents, whereas the effects of shorter travel time will become more important for hydrolyzing constituents.

An independent review conducted by Allison Geoscience Consultants (Allison Geoscience Consultants, 1997b) of the probabilistic sensitivity analysis was performed for EPA OSW. This review reached the following conclusions:

- the sensitivity analysis met the objective of identifying the most important parameters in determining EPACMTP model output.

- an independent sensitivity analysis using a method that relied on linear and rank order correlation coefficients to estimate the performance in determining all of the model responses in a Monte Carlo simulation indicated that this method of ranking model input parameters yielded results similar to the probabilistic ranked difference method. The linear correlation coefficient results identify approximately the same parameters as being most important, although the relative importance is somewhat different.

- Spearman rank order sensitivity analysis results, which are probably a more appropriate ranking because of the non-linear relation between many of the input parameters and the model response also indicated similar parameters as being most important. The exception is the appearance of aquifer dispersivity in the ranking, which is not a parameter that is commonly known and will not be requested of the user.

- the similarities in both rank order analyses confirmed the results of the probabilistic differences method used to identify the most sensitive parameters.

Based on the combined results of each of the three sensitivity analyses, the Agency developed a list of the twelve most sensitive EPACMTP parameters for the industrial waste management scenarios considered for the Tier 2 analyses (Table 3-7). These twelve parameters were selected to develop the neural networks for each WMU (see Section 5) for the Tier 2 analysis. As will be described in Section 5, initial attempts to train on all twelve parameters were unsuccessful. However, accurate neural networks were developed using 6-7 EPACMTP input parameters as is described in Section 5.1

Table 3-7 Most Sensitive EPACMTP Input Parameters Based on the Combined Results of Deterministic and Probabilistic Sensitivity Analyses

Parameter Group	EPACMTP Input Parameter
Source Parameters	area (AREA)
	infiltration (SINFIL)
	ponding depth for surface impoundments (HZERO)
Chemical-Specific Parameters	hydrolysis rate (RLAM1)
	organic carbon partition coefficient (KOC)
Unsaturated Zone Parameters	unsaturated zone thickness (DSOIL) - sensitive only for hydrolyzing and adsorbing chemicals
	percent organic matter in the unsaturated zone (POM)
Saturated Zone Parameters	aquifer thickness (ZB)
	hydraulic conductivity of saturated zone (XKX)
	fraction organic carbon in the saturated zone (FOC)
	hydraulic gradient (GRADNT)
Well Parameters	distance to well (RADIS)
	angle of well off the contaminant plume centerline

4.0 CALCULATION OF THE TIER 1 LEACHATE CONCENTRATION THRESHOLD VALUE (LCTVs)

This section describes the method used to compute the Tier 1 National Evaluation LCTVs, including the assumptions and EPACMTP input parameters used (Section 4.1), the calculation of DAFs that are used to develop Tier 1 LCTVs (Section 4.2), and the determination of Tier 1 LCTVs (Section 4.3). EPACMTP was run using nationwide distributions of input parameters and some conservative assumptions to determine the 90th percentile DAF for each chemical on the list of Industrial Waste chemicals of concern. This section includes a description of the assumptions and input parameters used to compute Tier 1 LCTVs.

4.1 Assumptions and Parameters

Many of the assumptions used in other Agency applications of EPACMTP were used to develop Tier 1 LCTVs, including the nationwide empirical data used to characterize WMUs and the saturated and unsaturated zones at waste management facilities (U.S. EPA, 1987). The reader is referred back to Section 3.3 of this document for an overview of the modeling assumptions and to previously developed background documents for EPACMTP (U.S. EPA, 1996a, 1996b, and 1996c) for additional details on the development and application of EPACMTP. Additional modeling assumptions that are similar to other EPA applications include:

- The time period during which contaminant migration was modeled was 10,000 years.

- The leachate pulse duration for landfills was modeled as a finite-source controlled by the ratio between initial contaminant mass in the landfill and the annual mass removed by leaching.

- In the case of surface impoundments, waste piles and land application units, the leachate pulse duration has taken to be the same as the unit's operating life, as follows:

  - Surface impoundment: 20 years
  - Waste pile: 20 years
  - Land application unit: 40 years

  It was assumed that any waste remaining at the time the units are closed, is either removed or has negligible additional contribution to leaching.

- Rather than running EPACMTP for 2,000 simulations for each of 175 organic chemicals, EPACMTP was run for a selected number of values of hydrolysis rate (?) and retardation factor (R). Then for chemicals whose ? and R fell in between these values, an

interpolation procedure was used to determine the constituent's DAF. This technique reduced the computational effort required wile maintaining the desired accuracy.

- A separate series of simulations were performed for each of the non-linear metals, given the required difference in the modeling methodology used to model the monitoring well concentration of metals as a function of its leachate concentration.

The major differences between other previous EPA applications of EPACMTP and the assumptions used for the Tier 1 analyses are: 1) in addition to computing infiltration for the no-liner scenario for all four WMUs, infiltration from the WMU was computed for single-liner and composite-liner scenarios for landfills, waste piles, and surface impoundments and 2) rather than allowing the monitoring wells to be located within plus or minus 90E of the plume centerline, the monitoring wells were located 150 m downgradient on the plume centerline. These assumptions were based on agreements reached by the Association of State and Territorial Solid Waste Management Officials (ASTSWMO) Steering Committee, consisting of representatives from the states and EPA. The details of the differences in these assumptions are discussed in the following sections.

Assumptions Used to Calculate Infiltration Rates

The Tier 1 analyses are designed to allow a user to select the most appropriate type of WMU liner from three liner scenarios for landfills, surface impoundments, and waste piles (land application units consider only the no-liner scenario). The assumptions used to compute infiltration rates for each of the three liner scenarios for all four WMUs are summarized in Tables 4-1 through 4-4.

Infiltration rates were computed with the HELP model (see Section 3.1) for two liner scenarios: the no-liner scenario, consisting of a WMU that is developed on underlying native soils and the single-liner scenario, consisting of a single two-foot thick clay liner (refer back to Figure 2-2). Infiltration rates for the composite-liner scenario, consisting of a clay liner with a flexible membrane liner (FML) on top of the clay layer were computed using a liner leakage equation developed by Bonaparte et al (1989) to estimate leakage through pinholes in a geomembrane for good contact conditions:

$$Q = 0.21 \cdot a^{0.1} \cdot h_W^{0.9} \cdot k_S^{0.74}$$

where: Q = rate of leakage through a circular hole in the geomembrane component of the composite liner (m^3/s)
a = geomembrane hole area (m^2)
h_W = head of liquid on top of the geomembrane (m)

k_S = hydraulic conductivity of the low-permeability soil component of the composite liner (m/s)

The specific assumption regarding hole size and frequency of holes are listed in Tables 4-1 through 4-3. Further details of the liner leakage modeling are provided in Appendix B.

Ground-Water Well Assumptions

Two parameters used to determine the location of the downgradient ground-water monitoring well were set to constant values to approximate a conservative scenario for well location. The downgradient distance to the well was set to a constant value of 150 m from the boundary of the WMU and the angle of the monitoring well off of the leachate plume centerline was set to 0^o (Figure 4-1). Each state reserves the final authority on the location of ground-water wells. However, for the national Tier 1 evaluation, the location was set to a conservative distance of 150m.

4.2 Determination of Dilution Attenuation Factors (DAFs)

To calculate the Tier I LCTVs, the EPACMTP model is run for 2,000 iterations (2,000 sets of random selections of parameter values) for each chemical. The output of each simulation, the ground-water concentration is converted to a DAF and the 2,000 values are ranked from highest to lowest to form a cumulative probability density function (PDF). The 90^{th} percentile lowest DAF is selected from this PDF (Figure 4-2).
DAFs were determined for all chemicals except for those metals that exhibit non-linear sorption (see Section 3.2). As is described in Section 3.2, the ground-water well concentrations of the non-linear metals is dependent upon the initial concentration of metals (leachate concentration) and the total concentration of metal in the subsurface. A DAF is not calculated for non-linear metals, per se. A back calculation is performed to determine the initial leachate concentration for which 90% of the simulations results in a ground-water well concentration that does not exceed the toxicity reference level (MCL or HBN). This is the equivalent of computing a 90^{th} percentile DAF.

4.3 Calculation of Leachate Concentration Threshold Values (LCTVs)

To develop liner-specific LCTVs for the chemicals of concern, the DAF is multiplied either by the maximum contaminant (MCL), or the health-based number (HBN). For chemicals with hydrolysis daughter products the MCL or HBN of the most toxic daughter compound (the lowest MCL or HBN) is used to compute the LCTV.

Table 4-1 Assumptions Used to Compute Infiltration for Landfills

	No Liner	Single Liner	Composite Liner
Method	HELP model simulations to compute an empirical distribution of infiltration rates for a 2 ft. thick cover of three native soil types for 97 nationwide climate stations represented by 30 climate classes. Infiltration rates for a specific site were obtained by using the infiltration rate for the nearest climate station.	HELP model simulations to compute an empirical distribution of infiltration rates through a single clay liner for 97 nationwide climate stations represented by 25 climate classes. Infiltration rates for a specific site were obtained by using the infiltration rate for the nearest climate station.	Bonaparte et al (1989) Liner Leakage Equation (See Appendix B).
Final Cover	Monte Carlo selection from distribution of soil types. 2 ft thick native soil (1 of 3 soil types: silty clay loam, silt loam, and sandy loam) with a range of mean hydraulic conductivities ($4.7x10^{-6}$ cm/s to $6.4x10^{-4}$ cm/s).	3 ft thick clay cover with a hydraulic conductivity of $1x10^{-7}$ cm/sec and a 10 ft thick waste layer. On top of the cover, a 1 ft layer of loam to support vegetation and a 1 ft drainage layer.	No cover modeled. DAFs for composite liner are already high with a liner only and the geomembrane is limiting factor in determining infiltration.
Liner Design	Assumes no liner beneath waste.	3 ft thick clay liner with a hydraulic conductivity of $1x10^{-7}$ cm/sec. Assumes constant infiltration rate (assumes no increase in hydraulic conductivity of liner) over modeling period.	3 ft thick clay liner with a hydraulic conductivity of $1x10^{-7}$ cm/sec, 1 ft hydraulic head, 40 mil HDPE FML geomembrane w/ small holes (0.005 in^2), one hole per acre, "good" field conditions, and good contact between the liner and soil. Assumes same infiltration rate (i.e., no increase in hydraulic conductivity of liner) over modeling period.
Infiltration Rate	Monte Carlo selection from an empirical distribution of values: min=$1x10^{-5}$ m/yr med=0.13 m/yr max=1.08 m/yr	Monte Carlo selection from an empirical distribution of values: min=0.0 m/yr med=0.043 m/yr max=0.053 m/yr	Constant value: $3.41x10^{-5}$ m/yr

Table 4-2 Assumptions Used to Compute Infiltration for Surface Impoundments

	No Liner	Single Liner	Composite Liner
Method	Darcy's Equation for infiltration through a single sludge/native soil layer with a Monte Carlo selection of ponding depth from the nationwide OPPI survey of surface impoundments.	Darcy's Equation for infiltration through a single clay liner with a Monte Carlo selection of ponding depth from the nationwide OPPI survey of surface impoundments.	Bonaparte et al (1989) Liner Leakage Equation (See Appendix B).
Ponding Depth	Based on Monte Carlo selection from nationwide distribution of ponding depths.	Based on Monte Carlo selection from nationwide distribution of ponding depths.	Assumes a 10 ft ponding depth.
Liner Design	1 ft to 3 ft thick layer of sludge/native soil in the bottom of the impoundment. Monte Carlo selection from distribution of hydraulic conductivity values for this layer ranging from $1x10^{-7}$ cm/s to $1x10^{-5}$cm/s. Waste is removed after 20 years and no final cover is installed.	3 ft thick clay liner with a hydraulic conductivity of $1x10^{-7}$ cm/sec. No leachate collection system. Single clay liner. Assumes no increase in hydraulic conductivity of liner over modeling period. Waste is removed after 20 years and no final cover is installed.	3 ft thick clay liner with a hydraulic conductivity of $1x10^{-7}$ cm/sec, 40 mil HDPE FML geomembrane w/ small holes (0.005 in^2), one hole per acre, "good" field conditions, and good contact between the liner and soil. Assumes constant infiltration rate (i.e., no increase in hydraulic conductivity of liner) over modeling period. Waste is removed and no final cover is installed. Geomembrane liner is limiting factor that determines infiltration rate.
Infiltration Rate	Calculated based on Monte Carlo selection of ponding depth from an empirical distribution of values. The resulting distribution of infiltration rates is: min=$1.8x10^{-2}$ m/yr, med=3.94 m/yr, max= 89.6 m/yr.	Calculated based on Monte Carlo selection of ponding depth from an empirical distribution of values. The resulting distribution of infiltration rates is: min= $6.83x10^{-3}$ m/yr, med=$9.12x10^{-2}$ m/yr, max= 1.46 m/yr.	Constant value: $3.1x10^{-4}$ m/yr

Table 4-3 Assumptions Used to Compute Infiltration for Waste Piles

	No Liner	Single Liner	Composite Liner
Method	HELP model simulations to compute distribution of infiltration rates for a 2 ft thick layer of three native soil types for 97 nationwide climate stations represented by 30 climate classes. Infiltration rates for a specific site were obtained by using the infiltration rate for the nearest climate station.	HELP model simulations to compute distribution of infiltration rates through a single clay liner for 97 nationwide climate stations represented by 25 climate classes. Infiltration rates for a specific site were obtained by using the infiltration rate for the nearest climate station.	Bonaparte et al (1989) Liner Leakage Equation (See Appendix B).
Liner Design	Assumes no liner. Infiltration computed for three native soil types with hydraulic conductivity similar to range of waste hydraulic conductivities ($4.7x10^{-6}$ cm/s to $6.4x10^{-4}$ cm/s). Assumes waste is removed after 20 yrs and no final cover is installed.	3 ft thick clay liner with a hydraulic conductivity of $1x10^{-7}$ cm/sec, no leachate collection system, and a 10 ft thick waste layer. Assumes no increase in hydraulic conductivity of liner over modeling period. Assumes waste is removed after 20 yrs and no final cover is installed.	3 ft thick clay liner with a hydraulic conductivity of $1x10^{-7}$ cm/sec, 1 ft hydraulic head, 40 mil HDPE FML geomembrane w/ small holes (0.005 in^2), one hole per acre, "good" field conditions, and good contact between the liner and soil. Geomembrane is limiting factor in determining infiltration rate. Assumes waste is removed after 20 yrs and no final cover is installed.
Infiltration Rate	Monte Carlo selection from an empirical distribution of values: min=$1x10^{-5}$ m/yr med=0.17 m/yr max=1.08 m/yr	Monte Carlo selection from an empirical distribution of values: min=0.0 m/yr med=0.126 m/yr max=0.135 m/yr	Constant value: $3.41x10^{-5}$ m/yr

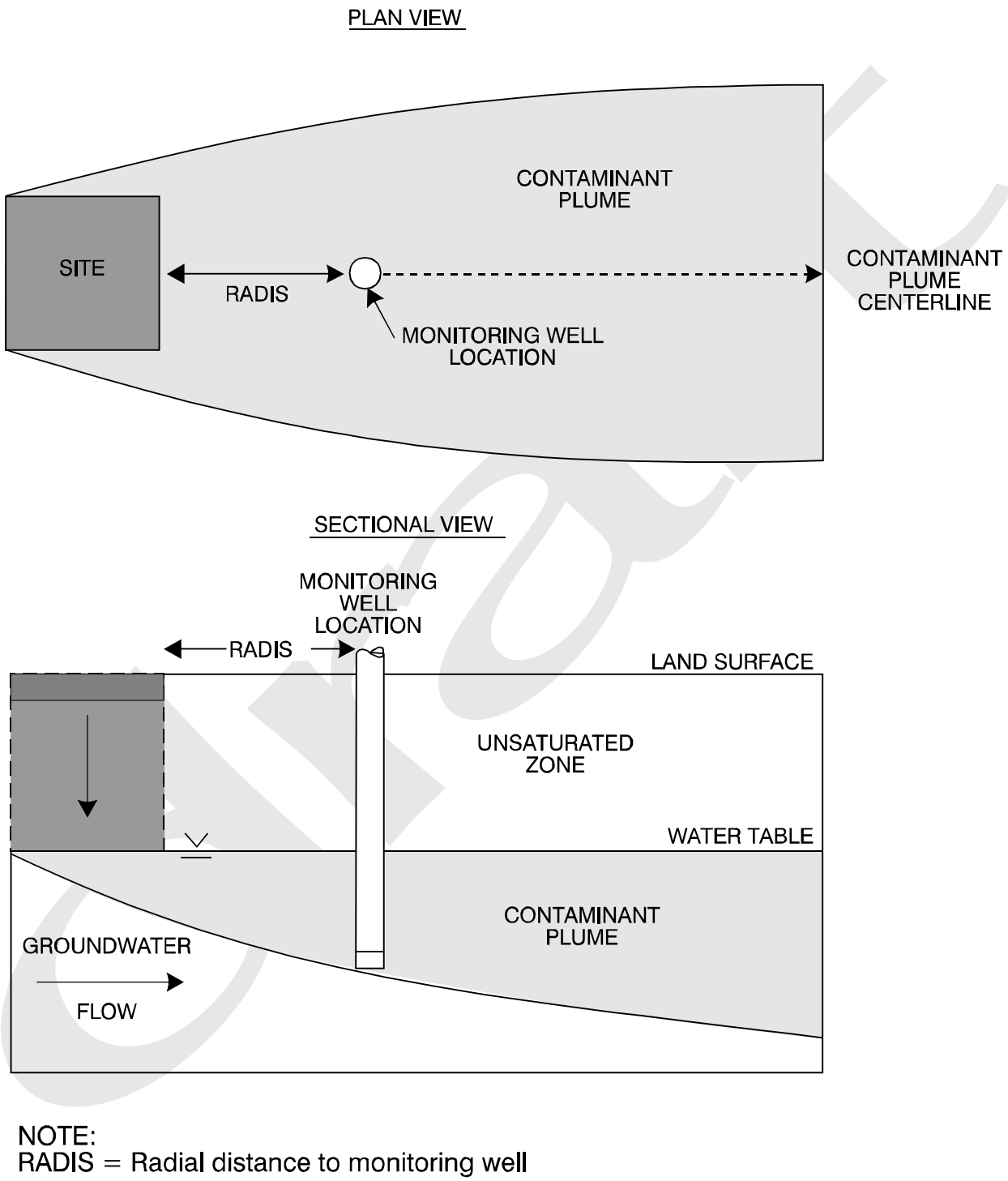

Figure 4-1 Well Location Parameters Used in the Tier 1 Analysis.

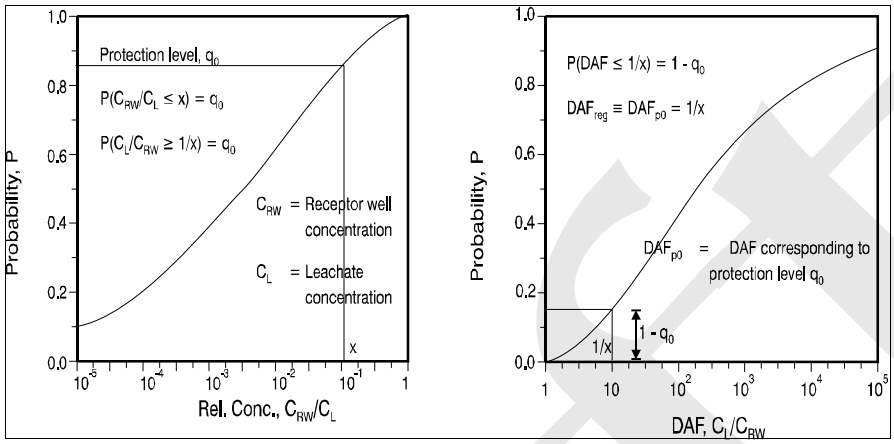

Figure 4-2 Cumulative Probability Density Functions of Ground-water Well Concentrations and DAFs

The LCTV for any constituent is capped at 1,000 mg/L. Therefore, if the LCTV calculated based on the DAF and the toxicity reference level is greater than 1,000 mg/L, the LCTV will be set to 1,000 mg/L. The Agency invites comments on whether leachate from industrial WMUs are likely to exceed 1,000 mg/L and if so, under what circumstances.

For the 39 constituents that determine whether a waste is characteristically toxic under 40 CFR 261.24 (U.S. EPA, 1990a), the LCTV is capped at the regulatory level for each constituent (Table 4-4). Any waste with leachate concentrations equal to or greater than the regulatory level is a hazardous waste under the RCRA and state laws.

Table 4-4 Toxicity Characteristic Regulatory Levels (U.S. EPA, 1990)

Chemical	Toxicity Characteristic Regulatory Level (mg/L)
Arsenic	5.0
Barium	100
Benzene	0.5
Cadmium	1.0
Carbon Tetrachloride	0.5
Chlordane	0.03
Chlorobenzene	100
Chloroform	6.0
Chromium	5.0
o-Cresol	200
m-Cresol	200
p-Cresol	200
Cresol	200
2,4-D	10.0
1,4-Dichlorobenzene	7.5
1,2-Dichloroethane	0.5
1,1-Dichloroethylene	0.7
2,4-Dinitrotoluene	0.13
Endrin	0.02
Heptachlor	0.008
Hexachlorobenze	0.13
Hexachloro-1,3-butadiene	0.5
Hexachloroethane	3.0
Lead	5.0
Lindane	0.4
Mercury	0.2
Methoxychlor	10.0
Methyl ethyl ketone	200.0
Nitorbenzene	2.0
Pentachlorophenol	100.0
Pyridine	5.0
Selenium	1.0
Silver	5.0
Tetrachloroethylene	0.7
Toxaphene	0.5
Trichloroethylene	0.5
2,4,5-Trichlorophenol	400
2,4,6-Trichlorophenol	2.0
2,4,5-TP Acid (Silvex)	1.0
Vinyl chloride	0.2

5.0 DEVELOPMENT OF NEURAL NETWORKS FOR TIER 2 EVALUATION OF THRESHOLD VALUES

As stated in Section 1 of this document, to support the Tier 2 analysis, the Agency developed a user-friendly tool that is midway between a Tier 1 analysis and a Tier 3 comprehensive site-specific, data-intensive analysis. The Agency evaluated methods to develop a simplified approximation of a ground-water model that focuses on the most sensitive ground-water modeling parameters, allows the user to evaluate the effects of some WMU- or location-specific parameters, produces instantaneous results, and does not require a great deal of ground-water modeling expertise to use. During the course of its evaluation, the Agency determined that neural networks (described in Section 2.3) can and have been successfully used in ground-water modeling problems (Johnson and Rogers, 1995) and would be the most appropriate predictive tool for the Tier 2 analysis.

This section describes how neural networks were used to develop a simplified tool that would emulate the EPACMTP ground-water analysis of liner designs using a subset of the most sensitive parameters and how they have been developed and applied to Tier 2 analysis of WMU liner designs. Section 5.1 describes how the key EPACMTP input parameters were selected for training neural networks. The assumptions and EPACMTP parameters included in the neural network training are presented in section 5.2. Section 5.3 describes the process of training the neural networks and how they were developed. Section 5.4 demonstrates how well the neural networks predict EPACMTP modeling results and describes the uncertainty involved in the use of the Tier 2 neural networks. Finally, Section 5.5 describes how neural networks developed for each of the four WMUs were integrated into one user-friendly Windows-based graphical user interface (GUI).

5.1 Sensitivity Analysis to Identify Key Parameters

As explained in Section 2.3 of this document, neural networks are used to approximate processes in the same manner as regression analysis, in which a number of independent parameters (inputs) are used to predict values of one or more observed dependent parameters (outputs). Therefore, the first step in developing neural networks to approximate EPACMTP was to determine an appropriate set of EPACMTP input parameters that would be used to predict the outcome of EPACMTP, the concentration of a chemical in a downgradient ground-water well used for drinking water and its inverse the DAF.

As was stated in Section 3.3.3, EPACMTP uses 52 input parameters to perform a ground-water modeling simulation. However, 24 of these parameters are either constant values, internally derived from other parameters, or are inactive for the scenarios of interest to this analysis. Therefore, the desired number of parameters on which to train the neural networks was a subset of the most sensitive of the remaining 28 parameters, preferably parameters that generally would

be known with a high degree of certainty at a particular facility and would have the most impact on the expected concentration of chemicals in a downgradient ground-water well.

To determine which parameters on which to train the neural network, sensitivity analyses evaluated the change in EPACMTP output, the ground-water concentration, as a function of changes in each of EPACMTP's input parameters for a landfill scenario (see Section 3.3.3). The deterministic and probabilistic sensitivity analyses identified the ten to twelve (depending on the WMU of interest) parameters that were ranked as the most sensitive parameters for the majority of modeling scenarios for the two-tiered approach (refer back to Table 3-7).

- EPACMTP has 52 input parameters
- 24 parameters are constant, dependent or not used
- Of the 28 remaining parameters, the Agency identified the top 12 most sensitive parameters for Industrial solid waste modeling scenarios
- Of the top 12 parameters, 7 were identified that represent the most sensitive parameters that can be used to develop a robust neural network.

Initially, the following 10 EPACMTP parameters were selected to develop neural networks:

- waste area,
- infiltration rate,
- chemical-specific organic carbon partition coefficient,
- chemical-specific decay rate,
- the product of the percent organic matter in the unsaturated zone times fraction organic carbon in the saturated zone,
- the product of hydraulic conductivity (m/yr) and hydraulic gradient (m/m)
- depth to water table,
- aquifer thickness,
- angle of the monitoring well off of the plume centerline, and
- distance to the monitoring well.

Several attempts to develop neural networks with this number of parameters indicated that it was possible to develop neural networks with a high coefficient of determination (R^2). However, because of the combined non-linearities in EPACMTP and complexities in the resulting output of the EPACMTP (i.e., the response surface), the numbers predicted by the Tier 2 neural networks were often inaccurate. They would differ from the actual EPACMTP result by at least an order of magnitude in many cases. This was most likely a result of the wide variation in output values, up to several orders of magnitude. Therefore, an evaluation was performed to determine the optimum number of EPACMTP input parameters that could be used to train neural networks with the required accuracy. This evaluation indicated that seven EPACMTP input parameters could be used to develop accurate neural networks for each of the four WMUs for the Tier 2 analyses:

- waste area,
- infiltration rate,
- chemical-specific K_{OC} (for surface impoundments, waste piles, and land application units),
- chemical-specific decay rate,
- depth to water table,
- aquifer thickness, and
- distance to the monitoring well

The landfill modeling analyses for Tier 2 consider large waste volumes and assume an essentially steady-state source scenario. As a result, K_{OC} becomes an insensitive parameter (K_{OC} has no effect on the well concentration under steady-state conditions). Modeling the other three WMUs considered each of the seven parameters listed.

5.2 Assumptions and Parameters Used to Develop Neural Networks

Once the most sensitive parameters were identified, the assumptions and the modeling scenarios that would be considered in the Tier 2 analyses were delineated. The modeling scenarios were essentially similar to those used to develop the Tier 1 LCTVs (see Section 4.0). EPA used the neural network training software package NNModel version 3.2, to develop neural networks for the Tier 2 evaluation. Feed-forward, backpropagation neural networks with one hidden layer were designed for this investigation. The input layer consisted of six units for landfills and seven units for the other three WMUs, with each unit representing each input parameter (area, infiltration, K_{OC}, decay rate, depth to water table). The output layer consisted of the ground-water well concentration which are then converted to a DAF. See Figure 5-1 for a schematic diagram of the neural network structure for surface impoundments, waste piles, and land application units).

The hidden layer initially consisted of one neuron, which is automatically incremented by the neural network training software to a maximum of 35 hidden neurons. Training was performed for 10,000 to 20,000 iterations, and a conjugate gradient optimization, a method of adjusting the weights, was performed to minimize the errors. The neural network training software provided summaries of the training statistics at the end of the training session.

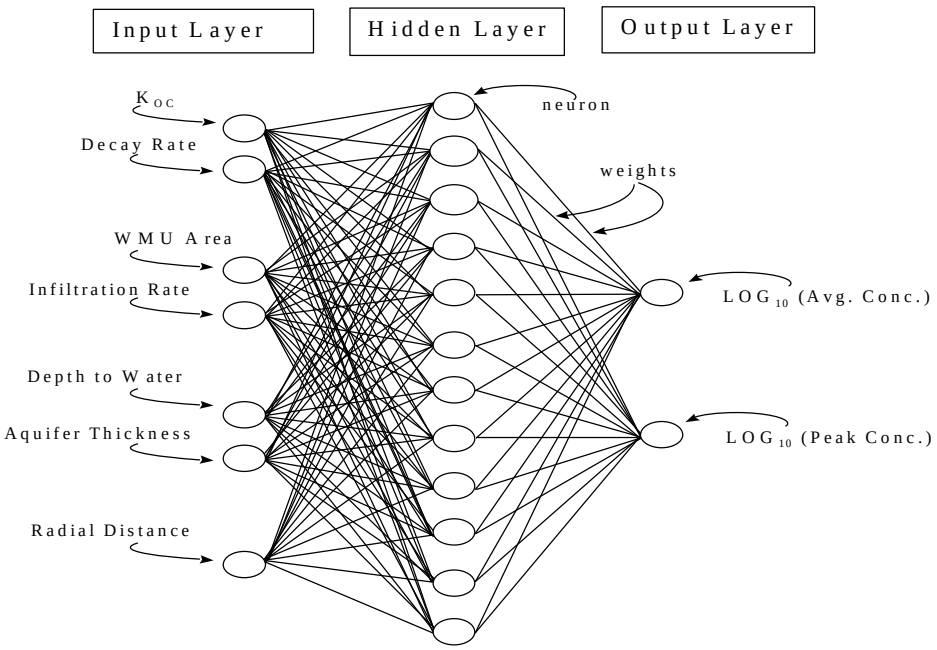

Figure 5-1 Diagram of Neural Network for EPACMTP Model (Parameters)

The trained network was first tested by evaluating its performance against the training set, to see how well it learned the training data matrix. The network was then tested against data is had not seen before, to evaluate its generalized performance. The trained and tested neural network was then converted into a simple computer code in the C programming language. This program was then compiled into an executable file that can be run as a user-friendly stand-alone executable program.

5.3 Neural Network Development

The results of EPACMTP simulations were collected in spreadsheets in one initial data matrix. To follow the network learning progress from the beginning of the training, a training data set was coupled with a test data set. Additional data sets were created parallel to the network training and were appended to or replaced with the current training and/or test data set depending on training requirements. The details of this process for the neural networks developed for each WMU are described in Appendix A.

Each data set consisted of a series of EPACMTP input and output parameter values, with each row consisting of a combination of input values and the resulting EPACMTP output values. A column represents one input parameter, one row represented an input parameter combination, and each cell contained an input parameter value. Input parameters with values varying over several orders of magnitude (e.g. 10^{th} percentile of area=108, and the 90^{th} percentile of area=40500) were transformed to logarithmic values. This conversion was made for the following inputs: LAMBDA, KOC, AREA, and RADIUS. The other input parameters (SINFIL, DSOIL, and ZB) remained in their linear form. The values of the output parameters also varied over more than one order of magnitude and were converted to logarithmic values.

Development of each of the four neural networks required the use of three software systems. The training and test data were produced with EPACMTP, the data matrices were collated into spreadsheets, which were then imported into the neural network software package NNModel version 3.2 (Neural Fusion, 1998). Figure 5-2 gives an overview of this process. EPACMTP was run for 2000 iterations for each input file consisting of a unique combination of input values. The model simulated the leaching from each WMU type and calculated the corresponding peak and average 90^{th} percentile monitoring well concentrations, which were then imported to spreadsheets. The data sets in the spreadsheets were then imported into the neural network software. Internal neural network training parameters including the training method, number of training iterations, and the input parameter descriptors were defined and the neural network training was started. The process of training and testing the neural networks for each WMU is described in detail in Appendix A.

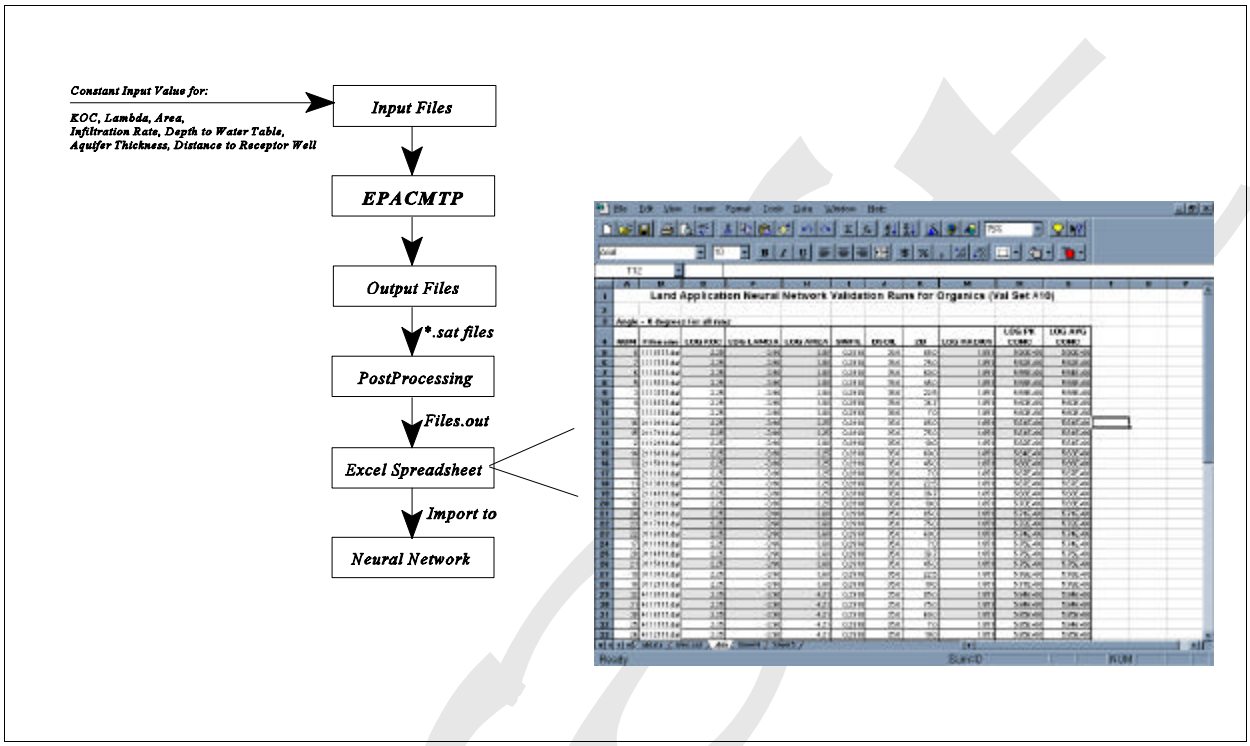

Figure 5-2 Overview of Neural Network Training Procedure

5.4 Neural Network Performance Evaluation

Following the iterative process of training and testing the neural networks for each WMU, their predictive ability was evaluated through an independent validation test. The final networks were used to predict monitoring well concentrations and DAFs for a comprehensive set of input parameters, which was generated independently from the data on which the networks were trained. The validation data sets were intended to resemble the site data that a user might enter into the neural network model. The validation data sets reflect values representative of real site data and were randomly selected within the domain of values used to train the neural networks. The same data were also used as input to EPACMTP and the performance evaluation consisted of comparing the neural network predictions to the actual EPACMTP results.

The results of the neural network validation are summarized graphically in Figures 5-3 through 5-6. These figures show the performance of the neural networks for each of the four WMUs.

The performance of the neural networks is summarized in Table 5-7. This table provides, for each network, the number of training and testing data sets used, the number of data points in the final validation test, and the linear correlation, expressed as the coefficient of determination (R^2), for actual (EPACMTP) and predicted concentration values.

The validation results for the landfill neural network are shown in Figure 5-3. The figure shows the comparison of EPACMTP and neural network-generated peak monitoring well concentrations for a total of 115 validation cases. The monitoring well concentrations are shown on a logarithmic scale. The EPACMTP model simulations were all performed using an (arbitrary) initial leachate concentration of 10^6 mg/L. The highest monitoring well concentration obtained also approaches this same value, i.e., it corresponds to the case where the concentration in the monitoring well is the same as the concentration in the leachate. For this case, the DAF is equal to 1.0.

For clarity in the presentation of results, the results are shown in ranked order, from the cases with the lowest monitoring well concentration to the highest. The figure demonstrates that the neural network performs best in the high range of monitoring well concentrations (i.e., low DAFS); the prediction of the neural network is poorest for those cases where the monitoring well concentration was the lowest .

As will be discussed below, generally better neural network performance was obtained for the other WMU neural networks which had gone through more extensive training/testing than the landfill neural network. Nevertheless, the landfill neural network met the criterion that the coefficient of determination, R^2, should equal or exceed 0.9 for both the training data set and the validation data set (Table 5-7). The relatively poorer prediction in cases of low monitoring well concentration (high DAF) was deemed acceptable because these cases correspond to situations where leachate from the waste unit will have relatively little impact on ground-water resources. Conversely, simulation cases of high monitoring well concentration correspond to situations where the WMU leachate may have a significant ground-water impact, and accuracy of the neural network is of greater concern.

Figure 5-4 depicts the validation results for surface impoundments. The same trends in predictive accuracy of the neural network as a function of monitoring well concentration that were observed in the landfill case, are also evident here. Interestingly, although the surface impoundment neural network visually does an overall better prediction job than the landfill network, the R^2 value for the validation test, is actually somewhat lower (Table 5-7). This may be attributed to the presence of a number of poor predictions in a small number of cases in the low concentration range.

Results for the waste pile and land application unit validation tests are shown in Figures 5-5 and 5-6, respectively. In both cases, the neural network shows very good prediction accuracy, and

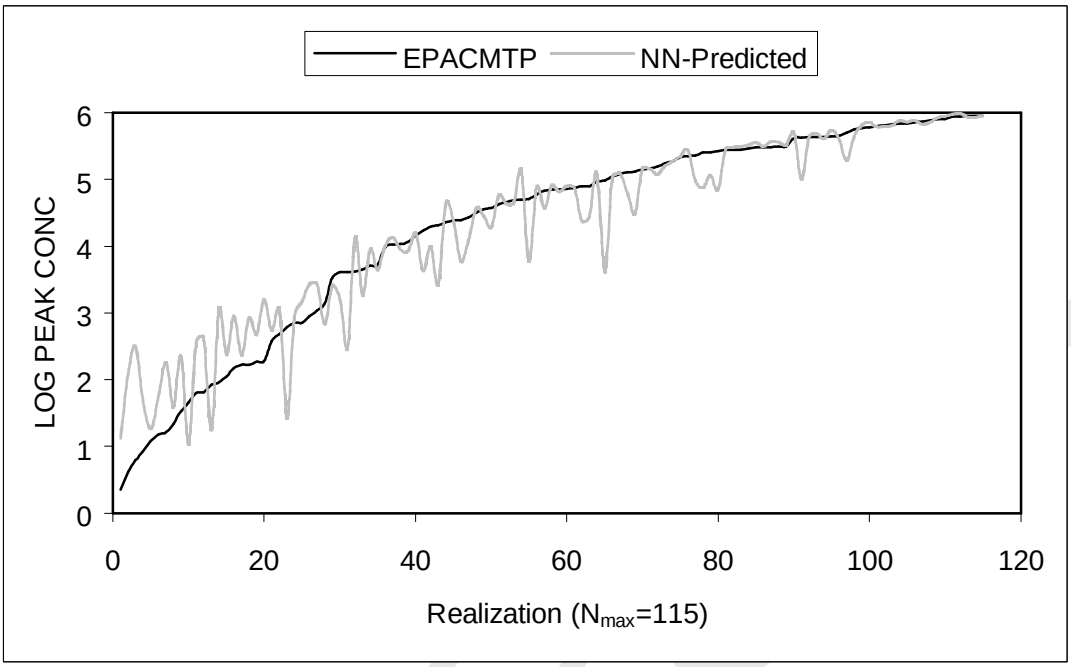

Figure 5-3 Comparison of EPACMTP Results and Neural Network Predictions of Peak Monitoring Well Concentration for Landfills.

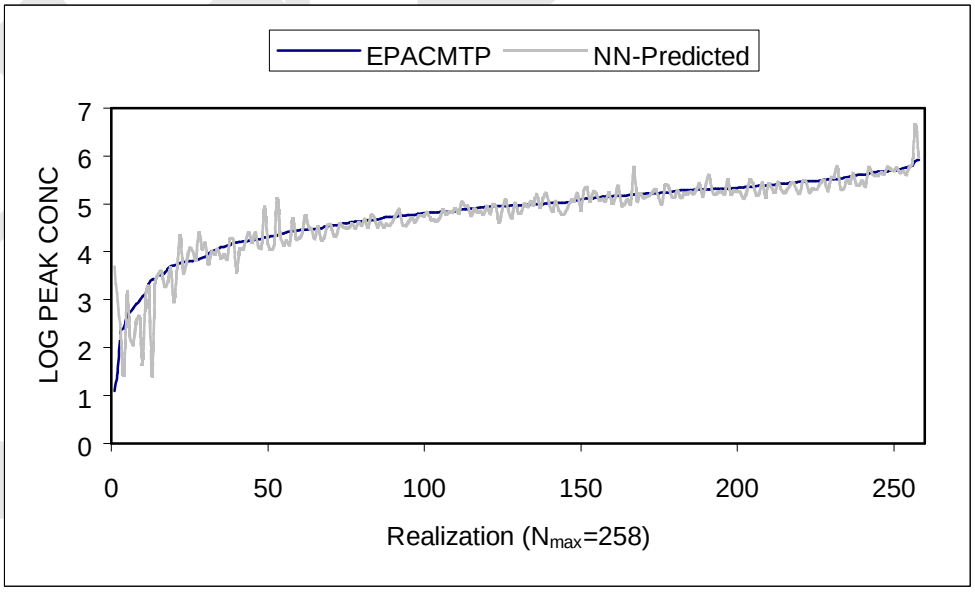

Figure 5-4 Comparison of EPACMTP Results and Neural Network Predictions of Peak Monitoring Well Concentration for Surface Impoundments.

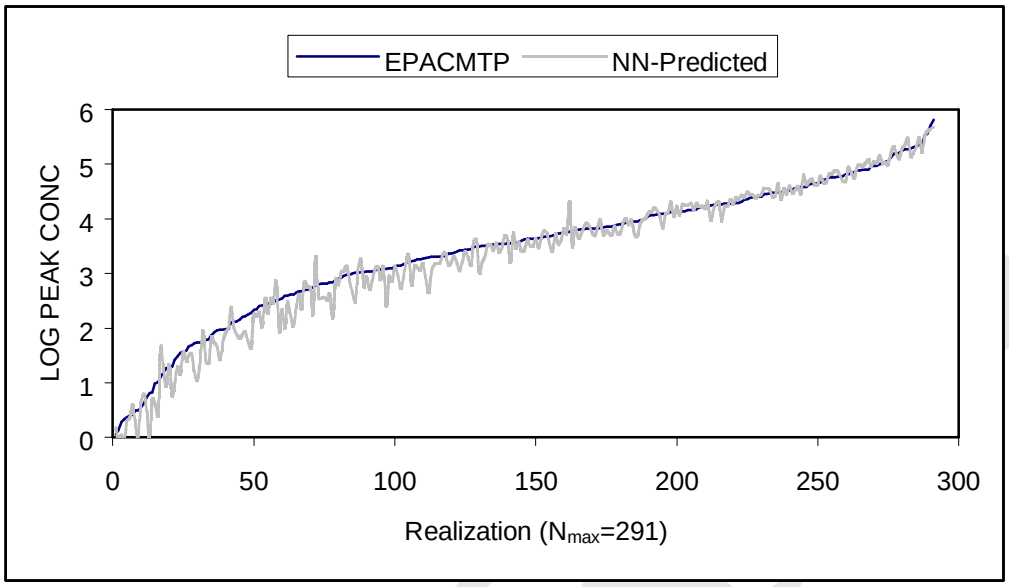

Figure 5-5 Comparison of EPACMTP Results and Neural Network Predictions of Peak Monitoring Well Concentration for Waste Piles.

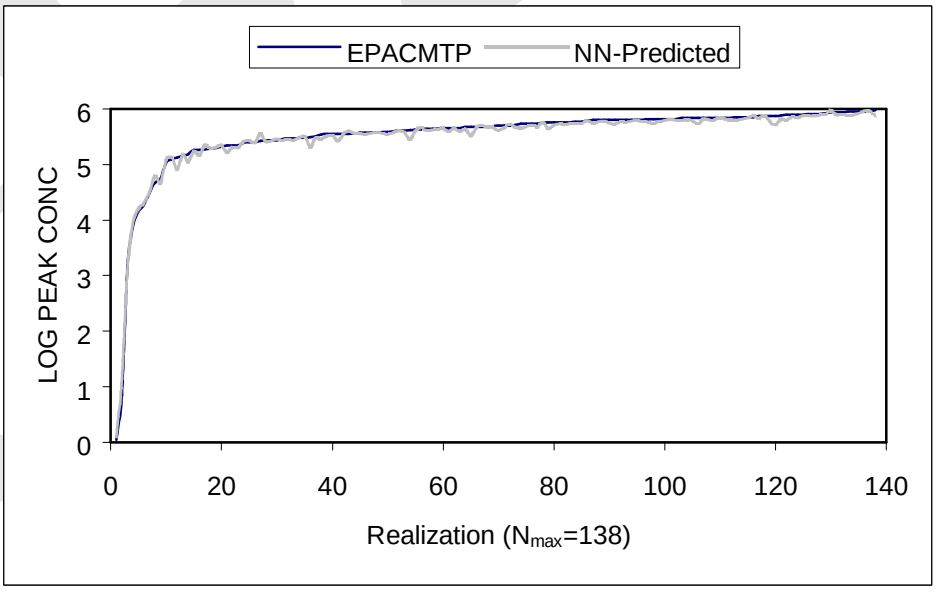

Figure 5-6 Comparison of EPACMTP Results and Neural Network Predictions of Peak Monitoring Well Concentration for Land Application Units.

Table 5-1 Neural Network Summary Statistics

Parameter	Landfill	Surface Impoundment	Waste Pile	Land Application Unit
Number of training/testing data sets	712	2,747	4,668	4,870
Maximum number of hidden neurons	10	20	32	34
Maximum number of nn iterations	31,000	388,399	160,082	120,073
Training R^2 (log peak conc.)	0.992	0.992	0.995	0.997
Number of validation data sets	115	253	291	138
Validation R^2 (log peak conc.)	0.902	0.825	0.978	0.994

correspondingly high R^2 values (Table 5-7). It may also be noted from this table that the number of training/testing data sets for the waste pile and land application unit networks were significantly greater than used for landfills and surface impoundments.

Collectively, the validation tests show good predictive ability for all four networks, with R^2 values equal to, or greater than 0.992. The comparison of landfill versus land application network results also indicates the incremental gains in predictive ability that may be realized through additional neural network training. The trained neural networks seem to give good generalized performance (i.e., they are able to predict the DAF to a high degree of accuracy for input values on which they have not been trained).

Uncertainty Assessment

Because the neural network is an approximation of EPACMTP, which is itself an approximation of real-world systems, the DAF values predicted by the neural network are inevitably subject to various sources of uncertainty. It is difficult to quantify the impacts of the various sources of uncertainty. The selection of a conservatively chosen DAF (i.e., 90^{th} percentile) is one way to reasonably ensure that the model predictions are appropriately protective in spite of uncertainty. A preliminary evaluation of the uncertainty associated with the neural network approximation of EPACMTP was done and is described in the *Draft Uncertainty/Sensitivity Analysis Background Document* (U.S. EPA, 1998).

Further investigation into the uncertainty associated with use of infiltration rates less than 0.001 m/yr revealed that constituents with a degradation rate or K_{OC} greater than zero gave monitoring well concentrations of zero, and were insensitive to infiltration rate. This suggests that the response surface that the neural network is intended to simulate has a discontinuity in it where the infiltration rates are low. This affirmed the difficulties in training the networks using low infiltration rates.

5.5 Integration of the Neural Networks into a Single User-Friendly GUI

Following the development of neural networks for each of the four waste management units, the predictive coefficients and software that make up each neural network were incorporated into one user-friendly Windows-based graphical user interface (GUI) that is used to perform both Tier 1 and Tier 2 analyses of WMU liner designs.

To verify that the GUI was passing the correct parameter values and computing DAFs in the same manner as each individual neural network was demonstrated to do, verification tests were performed on the GUI using sample data sets of input and output for each of the four neural networks. The results indicated that the neural networks in the GUI performed as expected.

6.0 APPLICATION OF MODEL RESULTS TO WASTE MANAGEMENT

The Tier 1 LCTV Look-Up tables discussed in Section 4.0 and the neural network approximation of EPACMTP have both been linked to a Microsoft Windows™-based graphical user interface. This user-friendly software package (IWEM) allows the user to enter chemical and facility information and determine if a proposed WMU will be considered protective of ground water. The use and interpretation of the Tier 1 and Tier 2 evaluations are described in this section (Sections 6.1 and 6.2, respectively).

6.1 Use and Interpretation of Tier 1 Evaluation

The potential impact that a WMU may have on ground-water resources is characterized by comparing the estimated waste constituent leachate concentration (TCLP or other appropriate leachate test method) to the calculated LCTV in the appropriate Look-Up Table. The result of this comparison determines the recommended liner system for the WMU or determines whether land application of this waste is appropriate (i.e., the waste constituent concentrations will not exceed health-based numbers at a down gradient ground-water well).

For example, if the leachate concentrations for all constituents are lower than the corresponding no-liner LCTVs, then no liner is recommended as being sufficiently protective of ground water. If any leachate concentration is higher than the corresponding no-liner LCTV, then a minimum of a single clay liner is recommended. If any leachate concentration is higher than the corresponding single-liner LCTV, then a minimum of a composite liner (an FML geomembrane overlain by a clay liner) is recommended. For waste streams with multiple constituents, the most protective liner that is specified for any one constituent is the recommended liner design.

An electronic version of these look-up tables is included in the IWEM software as the National Evaluation, and a printed copy of the tables are included in the Assessing Risk Section of the Ground-Water Protection section of the ***Guidance*** (Tables 4.1 to 4.4).

The IWEM software allows the user to enter the estimated leachate concentrations for waste constituents and compares these leachate concentrations to the corresponding LCTVs to recommend a liner design or determine whether land application is appropriate. The Tier 1 National Evaluation does not require site-specific data, and the resulting design recommendations are based solely on an evaluation of waste characteristics and national ground-water characteristics.

If the user is not satisfied with the recommendations of the National Evaluation or if site-specific conditions seem likely to support the use of a liner design different from the one recommended (or suggest a different conclusion regarding the appropriateness of land application of a waste), then

the user can proceed to the Location-Adjusted Evaluation (Tier 2) or conduct a site-specific ground-water fate and transport analysis (Tier 3).

6.2 Use and Interpretation of Tier 2 Evaluation

The neural networks developed for Tier 2 have been incorporated into the Industrial Waste Evaluation Model (IWEM) graphical user interface and are designed to provide the user flexibility in evaluating WMU designs. IWEM incorporates the neural networks for each of the four WMUs and is designed to provide a user-friendly software tool that allows users to input location-specific data for up to seven EPACMTP input parameters and quickly determine if a proposed WMU design will be protective of human health and the environment.

As with Tier 1, a list of chemicals commonly encountered in industrial waste is provided along with necessary chemical-specific data such as decay rate and sorption coefficients, as well as HBNS and/or MCLs. IWEM also allows the user to enter user-specified chemicals and required chemical property data, including user-specified TRLs. The user is requested to input location-specific data, where available, and to document the source of these data. If location-specific data are not available the Tier 2 evaluation provides default values that are based on representative nationwide data. Upon entering the required data, the user is provided with recommendations regarding whether or not a specific liner type for a WMU is protective based on the location-specific data, the modeling results, and on the TRLs for the chemicals of concern.

Similar to the Tier 1 analysis, the leachate concentration for each waste constituent is compared with the LCTV determined by the neural networks. If the user chooses to have the infiltration rate estimated by the model, then the results are presented in terms of two types of liners: no liner (in-situ soil) and single clay liner. These results are calculated from both MCLs and HBNs. If the leachate concentrations for all constituents are lower than the no-liner LCTVs, then no liner is recommended as being sufficiently protective of ground water. If any leachate concentration is higher than the no-liner LCTV, then at least a single clay liner is recommended. For waste streams with multiple constituents, the most protective liner that is specified for any one constituent is the recommended liner design.

If the user has a measured or calculated value for infiltration rate, that value can be directly entered as input for Tier 2. In this case, the user's expected leachate concentrations are compared to the LCTV calculated for this scenario. The modeling results are then presented to the user detailing whether the given scenario is recommended as being sufficiently protective of the ground water. These results are calculated for both MCLs and HBNs.

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